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Response surface study of a characteristic chemical plant

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RESPONSE SURFACE STUDY OF A CHARACTERISTIC

CHEMICAL PLANT

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ABSTRACT

Study of the return on investment response surface of a characteristic chemical plant indicates unimodality in the valid region, but the optimum design condition with this response surface is strongly affected by the correlation used for the investment. The method used for the design of this type of chemical plant incorporates the use of a simulation routine for preliminary estimates.

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I. INTRODUCTION

Recent literature (1,7,8,15,18,31,35) in the field of chemical engineering optimization is rich in the proposals of new and better algorithms. These articles concentrate on the application of a specific algorithm, however, and fail to use a realistic economic response surface. The only study known at present that used a realistic economic evaluation is that of Westerbrook (36), and this described only a single reactor.

The present study examines the response surface formed by the return on investment of an example chemical plant (Williams & Otto (38)). The effects of various parameter changes, including the investment correlation, were examined to determine the effects of these alterations on the economic objective function.

II. REVIEW OF LITERATURE

The plant utilized in this study was originally designed by Williams and Otto (38) to provide a generalized model for control studies. The process takes two raw materials into an isothermal, continuous stirred tank reactor where three coupled exothermic reactions occur to produce four other components, including the product, an intermediate. The reactor effluent is cooled and one component is removed by decantation before the other five components enter a distillation column for separation. The desired product is taken from the top of the column while the bottoms are split, part being sold as fuel and the remainder recycled to the reactor. Williams and Otto developed differential equations for each major piece of equipment and then solved them on an analog computer. The analog was allowed to reach steady state and then the return on investment was maximized by "trimming" the variable pots. The resulting parameter values were transferred to a digital computer with the reactor volume fixed. The accurate values for the optimum ROI of 30% were obtained by solving these equations by a fourth degree Runge-Kutta numerical integration (Kunz (23)), with incremental changes to the parameters. No sophisticated optimization technique was used to find the best operating point but they stressed that the plant was presented for control studies, not design.

Dibella and Stevens (8) described the plant completely in terms of steady state material balances derived from those originally developed by Williams and Otto (38). Their description contained nine equations and consisted of a material balance on each component, an overall material balance, a definition of the maximum separation possible in the distillation column, and an equation for the total flow out of the reactor. They first considered these as nine homogeneous equations and attempted to solve them by the steepest descent method. Once the solution to the system was determined, they described the equations as Taylor series expansions (Kaplan (20)) and linearized them by truncation. In addition to the nine describing equations, they added the objective function equation at this point and linearized it similarly by truncation of a Taylor series expansion. This system of ten linear equations was then solved by linear programming (Sasieni, Yaspan, Friedman (30)), the initial parameters were changed and the entire process repeated until they arrived at an optimum ROI of 73%.

A different approach to the plant solution was taken by Ahlgren and Stevens (1). They proposed to examine a direct search technique with the introduction of random error to represent errors in flow rate measurement. The technique they used (Kesten (21) and Kiefer and Wolfowitz (22)) normally evaluates the change of a variable as a constant times the sign of the slope. Ahlgren and Stevens (1) modified the objective function used by addition of a random variable to represent errors in the measurement of flow rates. The true optimum of their objective function, 46% ROI, had been located previously by a deterministic pattern search technique described in Wilde (37).

Henley and Rosen's (17) objective in using the plant was to demonstrate the convergence characteristics in building block model solutions, such as CHESS (Motard, Lee, and Barkley (27)). They used an initial estimate of the solution and then the true values calculated at this position were the next estimate. They utilized the Quasi-Newton method (Ayres (2)) which selects a base point and identity matrix initially to calculate a movement direction. As the search proceeded, the matrix was updated by secant approximations. At the solution, where the ROI was 109%, the matrix approximated the negative of the true Jacobian inverse. Otto (28) indicated that the true optimum was that reported by Henley and Rosen (17).

The significant result from these references for this thesis was that each of the four studies gave different values for the optimum. This suggests that the methods may differ in effectiveness, that the surface may have several local extremes, or that varying degrees of completeness in the objective function equation may result in different optimum locations.

III. DISCUSSION

A. PLANT DESCRIPTION

The plant to be studied is shown in Figure 1. Two pure raw materials A and B are fed into a perfectly mixed, isothermal, liquid phase reactor along with a recycle stream. In the reactor, three irreversible, coupled, exothermic, temperature dependent reactions occur to produce an intermediate C, the desired product P, an inert E, and a residual G according to the following reactions:

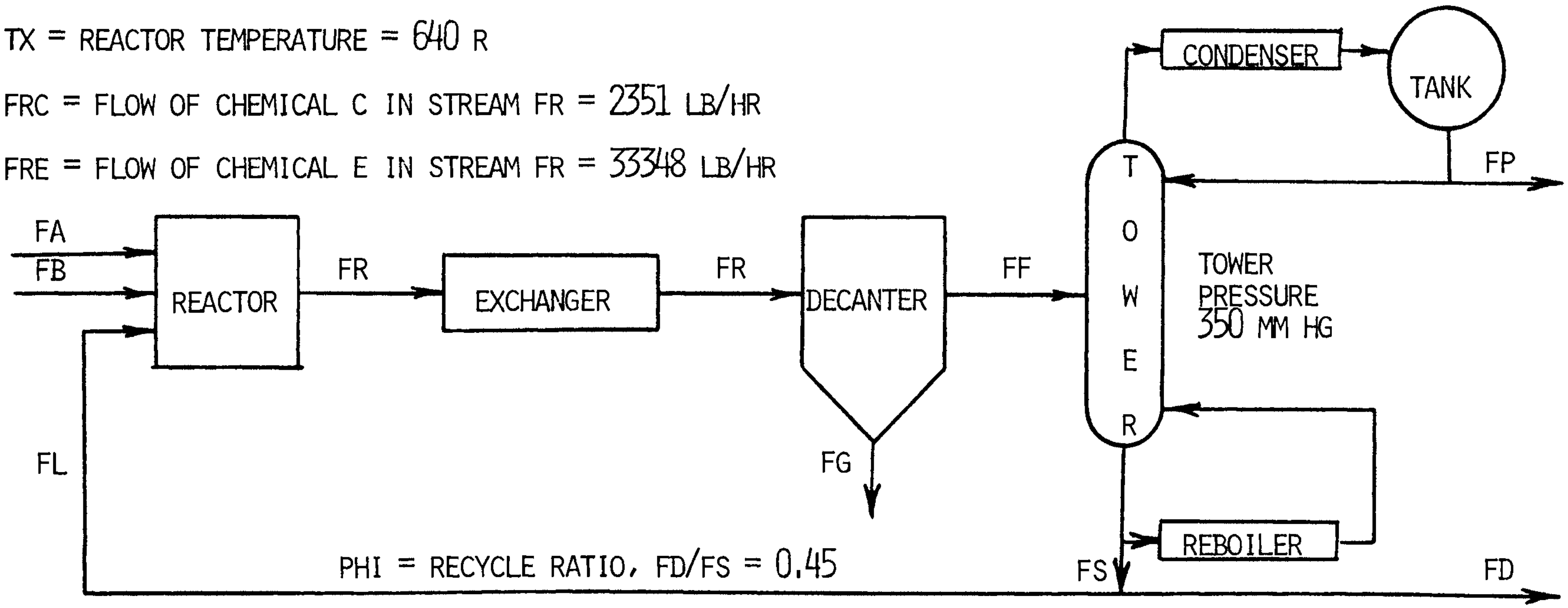
$$A + B \xrightarrow{k_1} C$$

$$C + B \xrightarrow{k_2} P + E$$

$$C + P \xrightarrow{k_3} G$$

The reactor effluent, consisting of all six components, is cooled in a reaction heat exchanger so that component G may be completely removed in a decanter. The distillation tower produces a fixed amount of overhead product, 40,000,000 pounds per year of pure P. The tower bottoms contain some P because of an azeotropic combination between P and E. These bottoms are split with a portion being sold for fuel and the remainder recycled to the reactor.

In this study, the original Williams and Otto Chemical Plant (38) was used as a base case from which to initiate the study of plant response surfaces. This plant was a combination of material balances and the algebraic expression for ROI (see Appendix A) using materials prices, the utilities directly related to the total flow rate out of the reactor, a constant investment, and constant indirect conversion and labor costs. It was felt that by using some simulation routine,



MASS BALANCE

STREAM / CHEMICAL	FA LB/HR	FB LB/HR	FR LB/HR	FG LB/HR	FF LB/HR	FP LB/HR	FS LB/HR	FD LB/HR	FL LB/HR
A	14502	0	11623	0	11623	0	11623	5230	6393
B	0	33325	36777	0	36777	0	36777	16550	20227
C	0	0	2351	0	2351	0	2351	1058	1293
E	0	0	33348	0	33348	0	33348	15007	18341
P	0	0	8098	0	8098	4763	3335	1501	1834
G	0	0	3719	3719	0	0	0	0	0
TOTAL	14502	33325	95916	3719	92197	4763	87434	39346	48088

FIGURE 1 WILLIAMS AND OTTO CHEMICAL PLANT

such as CHESS (27), a more realistic correlation could be made for the objective function (return on investment) by varying these factors. It was not possible, however, to verify the Williams and Otto plant investment and it became preferable to study the same process with more appealing unit sizes and costs, such as those suggested by CHESS-UMR (Gaddy, Gaines, and Doering (14)). This plant then became a second base case. Since each evaluation of the return on investment objective function necessitated a complete CHESS-UMR (14) run, at approximately two minutes per run, an algebraic representation of the second base case was established. Thus, there were two different plants considered with both an algebraic representation, and a CHESS-UMR simulation for each plant. In order to distinguish among the plants, they were designated:

A1 - Algebraic representation based on the Williams and Otto capitalization.

A2 - Algebraic representation based on the CHESS-UMR simulation.

C1 - Computer output representation based on the Williams and Otto capitalization.

C2 - Computer output representation based on the CHESS-UMR simulation.

B. RESULTS

1. Plant 1

a. Algebraic

The first objective was to verify the Williams and Otto calculations for plant A1 in order to develop plant C1. Examination of the article (38) proved that insufficient information was available for verification of all values (see Appendix

A). Correspondence with Otto (28) in St. Louis produced no additional information on the basic calculations and therefore it was assumed that discrepancies found in the original Williams and Otto article (38) were mistakes. After verifying the derivation of the equations for the plant, and using the modifications of Dibella and Stevens (8) and Christensen (5), the final model of plant A1 was defined as described in Appendix A. This definition of plant A1 consisted of thirteen nonlinear, steady state material balance equations in seventeen variables with seven inequality constraints, and the objective function as the return on investment:

$$ROI = \frac{(368FP + 8.4FD - 28FA - 42FB - 14FG - 0.37FR)}{V\rho} - 10$$

Where the F variables refer to the flow rates shown in Figure 1 and $V\rho$ is the total weight of the material in the reactor.

Utilizing Christensen's algorithm II-T, (see Appendix A), the entire system of fourteen equations has a straightforward solution procedure with the selection of only four design variables: FRC and FRE, the flows in pounds per hour of components C and E out of the reactor, TX the temperature in degrees R in the reactor, and PHI the recycle split. Because of this straightforward noniterative solution procedure to the system, it was convenient to place the system into an IBM 2741 remote computer terminal for an exhaustive examination. Using the immediate response of the remote computer terminal it was possible to conduct a thorough evaluation of the entire five dimensional hypersurface of the system as described. Evaluation of the results indicated that the objective function was more significantly affected by FRE and PHI than it was by FRC and TX, and further that the objective function was single valued in FRC and TX, or that sections of the objective function surface were similar for various values of FRC and TX. Thus it was possible to obtain a visual representation of the return on investment response surface as a function of two variables. This surface, shown in Figure 2 as contours of constant ROI for fixed FRC and TX, is characterized by a curved cliff generally approaching both axes asymptotically. Paralleling this cliff is another peninsula protruding into the valley formed by the cliff and the opposite wall. The top of the cliff slopes gently away from the precipice without further major topographical features. The valid region of the surface contains the optimum value of the ROI, 122%, and lies to the right of the positive definite constraint, R3 (the rate of reaction 3), and between the constrained A feed values. These constraints are those outlined by Christensen (5) and are discussed in Appendix A. The constrainton the feed, A, was originally suggested by Williams and Otto, and is actually more relevant to control studies than to design optimization. Inside the valid region, the cliff ridge passes from one feed constraint to the other with the maximum value between the two.

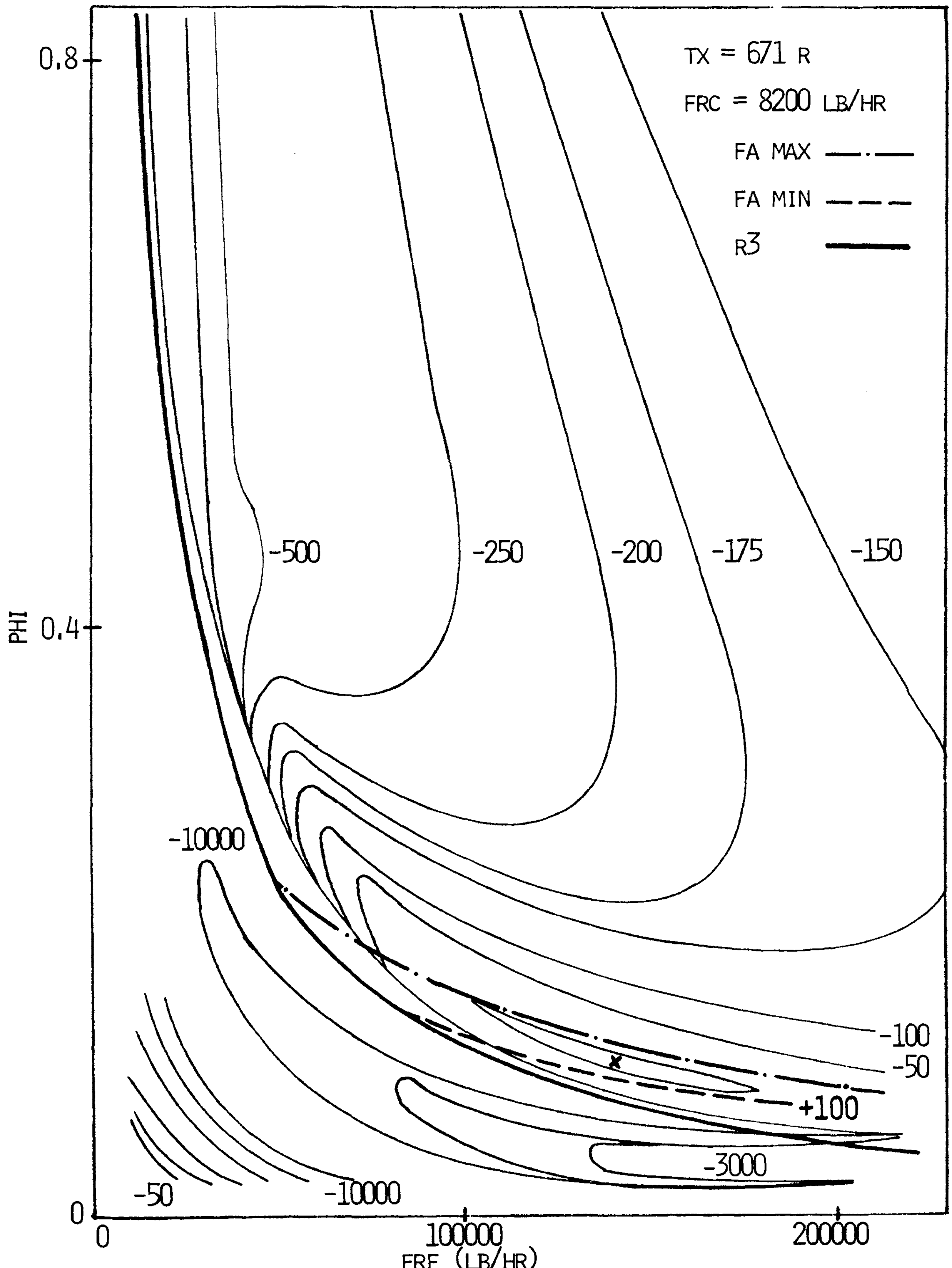


FIGURE 2 CONTOURS OF RETURN ON INVESTMENT - PLANT A1

Comparison of the various reported optimal solutions using the same ROI objective function led to discovery of yet a better optimal point which is the peak shown in Figure 2. Therefore, there were five different positions examined with plant A1, defined throughout the remainder of the study as follows:

WO = Williams and Otto (38)

DS = Dibella and Stevens (8)

AS = Ahlgren and Stevens (1)

HR = Henley and Rosen (17)

MN = Mason (present study)

TABLE I

COMPARISON OF REPORTED OPTIMUM - PLANT A1

	WO	DS	AS	HR	MN
TX(^{o}R)	640	656	636.5	657.64	671
FRC(lb/hr)	2350.6	3331	3420.56	7065	8200
FRE(lb/hr)	33348	60542	60677.76	111314	143570
PHI	0.45	0.24626	0.239	0.12964	0.101
ROI(%)	30.94	73.35	55.16	107.98	122.58

It must be noted that Ahlgren and Stevens used a different objective function and did, in fact, obtain the optimum of their function by a direct search technique.

The main objective of the previous studies was, in general, to promote a specific optimization technique. Thus, it appears that most selected the wrong plant to describe their techniques.

An attempt was also made to optimize plant A1 utilizing optimizing techniques not attempted by previous investigators. Both the Davidon (6) - Fletcher and Powell (13) and the Fletcher and Reeves (12) conjugate gradient methods were attempted with constraints added using the penalty functions suggested by Gottfried, Bruggink, and Harwood (16) (see Appendix D). These methods were attempted first using the programs in the IBM Scientific Subroutine Package. Then the Fletcher-Powell method was used as modified by Ferguson (10), again with constraints added using the Gottfried, Bruggink, and Harwood method. Finally, an attempt was made holding temperature and flow rate, FRC, constant, giving only a two dimensional problem. All of these methods failed to move away from the starting point substantially when started near the various reported optimum points. The results are shown in Table II. When the programs were run without constraints, the optimizing routine left the valid region and became stuck on the peninsula paralleling the cliff mentioned earlier.

Thus, in addition to the techniques proposed by Williams and Otto and Dibella and Stevens, other readily available optimization techniques failed to produce satisfactory results on this chemical plant. This strongly emphasizes the advantages of the direct search techniques used in this study and by Ahlgren and Stevens even though they are considered to be slow.

TABLE II

FORMAL OPTIMIZATION TECHNIQUES - PLANT A1

Program Used		Input				Return On Investment (%)	
Source	Method	FRE(lb/hr)	FRC(lb/hr)	TX(^{o}R)	PHI	Start	End
IBM	FMCG	60542	3331	656	0.25	70.23	72.00
ALF	FMFP	60542	3331	656	0.25	70.23	75.34
ALF	FMFP	60542	3331	656	0.24	75.46	75.48
ALF	FMFP	93000	7600	669.75	0.16	93.21	95.34
IBM	FMFP	93000	5300	669.75	0.16	107.20	109.03
ALF	FMFP	93000	5300	669.75	0.16	107.20	109.04
ALF	FMFP	113000	6250	673	0.13	118.25	118.41
ALF	FMFP	60542	3331*	656*	0.25	70.23	76.40
ALF	FMFP	66542	3331*	656*	0.22	78.67	78.67

*Variable held at constant value.

IBM refers to IBM Scientific Subroutine Package.

ALF refers to Ferguson modification (10).

FMCG refers to Fletcher-Reeves (12) method.

FMFP refers to Fletcher-Powell (13) method.

b. Numerical

Plant C1 was designed utilizing CHESS-UMR (14) in order to produce more realistic economics for the original Williams and Otto plant. See Appendix A for the details concerning the design. After plant C1 was found to approximate plant A1 at the Williams and Otto optimal conditions, several additional positions were checked to assure that this was a more than locally valid representation.

TABLE III

COMPARISON OF PLANTS A1 AND C1

INPUT	A1	C1
TX (^oR)	640.00	640.00
FP (lb/hr)	4763.00	4763.00
FRC (lb/hr)	2350.60	2350.60
FRE (lb/hr)	33348.00	33348.00
PHI	0.45	0.45
EQUIPMENT		
Fractionator		
Diameter (ft)	10.0	7.0
Height (ft)	40.0	38.4
Reflux Ratio	18.4	9.3
Velocity (ft/sec)	4.5	3.6
Heat Exchanger		
Area (ft^2)	569.0	810.0
Water flow (gal/hr)	184000.0	30209.0
Condenser		
Area (ft^2)	4260.0	3700.0
Water flow (gal/hr)	42600.0	36259.0
Reboiler		
Area (ft^2)	510.0	190.0
Steam flow (lb/hr)	8.8	14.0
Reactor		
Volume (ft^3)	92.8	92.8
ECONOMICS		
Investment	1035000	1025000
Working Capital	1745000	1723819
Total Capital	2780000	2749667
Revenue	13938300	13937736
Variable Costs	11054300	11098414
Fixed Costs	166000	174980
Other Costs	1769000	1770091
Operating Costs	13401000	13043485
Net Earnings	829000	894250
ROI (CHESS Calculations)	80.0	87.2
ROI (Williams & Otto)	30.1	32.5

Two cuts were made in the response surface above and below the indicated optimum with the results shown below:

TABLE IV

RETURN ON INVESTMENT CHARACTERISTICS - PLANT 1

TX (^oR)	640	640	640	640	640	640	640
FRC (lb/hr)	2350.6	2350.6	2350.6	2350.6	2350.6	2350.6	2350.6
FRE (lb/hr)	36000	36000	40000	50000	26461	33348	40000
PHI	0.3500	0.3845	0.3550	0.3500	0.4806	0.4500	0.4318
C1 ROI (%)	-137.0	21.1	41.9	37.6	-162.0	32.5	26.7
A1 ROI (%)	-172.3	24.7	40.9	12.0	-243.0	30.9	10.6

This indicates the cliff found in plant A1 is still present in C1 and the general contours are similar.

Plant 1 served its purpose by proving that a chemical plant described by a simulation routine, such as CHESS (27), contains the same general shape as that of an algebraic representation. Since the accuracy of the investment figures used by Williams and Otto could not be verified, there was a discrepancy for the heat required for the reactor (Appendix A), and the distillation tower was unusually sized, (10 ft by 40 ft), it was decided to go to an entirely new plant investment for the remainder of the study. This new plant was called C2.

2. Plant 2

a. Numerical

Plant C2 was composed of the same materials, component prices, flow rates, and equipment utilized in plant C1. The significant difference between plant C1 and C2 is the economic factors. Plant C2 utilizes the internal CHESS-UMR economic program with the exception of the ten factors specified in Appendix B. These economic factors affected the return on investment figures primarily in the utilities and Sales, Administration, Research, and Engineering (SARE) expenses, and in the investment. The major contributing factor toward the different investment was the Fenske (9)-Underwood (34)-Gilliland (15) distillation tower which ran approximately 25% of the total investment. The best R/R_{min} for the tower above was determined to be 1.2 as shown by the following results:

TABLE V.

OPTIMUM RATIO OF REFLUX - PLANT C2

R/R_{min}	1.01	1.03	1.05	1.07	1.10	1.20	1.50	3.00
ROI (%)	40.0	43.7	44.8	45.3	45.6	45.8	44.4	37.5

where T = 640°R, FRC = 2350.6 lb/hr, FRE = 33348 lb/hr and PHI = 0.45.

After the physical plant was completely determined, it remained to develop an algebraic expression for plant C2, since an algebraic expression is more rapidly evaluated than a complete CHESS-UMR run.

b. Algebraic

In order to establish an algebraic expression, plant C2 was operated at the previously reported optimal points (Williams and Otto, Dibella and Stevens, Ahlgren and Stevens, Henley and Rosen, Mason) since they include valid positions containing variations in all parameters. Table VI summarizes the results.

TABLE VI

ECONOMIC CHARACTERISTICS - PLANT C2

	WO	DS	AS	HR	MN
TX (^{o}R)	640	656	636.5	657.64	671
FRC (lb/hr)	2350.6	3331	3420.56	7065	8200
FRE (lb/hr)	33348	60542	60677.76	111314	143570
PHI	0.45	0.24626	0.239	0.12964	0.101
FR (lb/hr)	95915.0	157436.9	148435.50	281011.9	366774.4
Investment ($)	228035.75	266808.81	253571.31	323994.69	364570.50
Utilities ($/yr)	164664.05	254569.25	217445.93	405813.72	546465.89
ROI (%)	-29.97	49.56	201.04	86.40	28.39

No direct comparison between the results of plant 1 and plant 2 should be made because of the difference between the economic factors mentioned previously.

An examination of the investment and utilities costs for these runs indicated that they were both roughly 1.5 times FR, the flow out of the reactor in pounds per hour, which is the main plant flow rate. Since the object was to obtain a fast approximate estimate, it was decided to use this value to develop the algebraic expression. The algebraic expression developed and defined in Appendix B was:

$$ROI = \frac{(P' \cdot FP + D' \cdot FD - G' \cdot FG - A' \cdot FA - B' \cdot FB - U' \cdot FR - C')}{(E' \cdot FR)} - CC'$$

Using this algebraic expression with all constants as determined in Appendix B plus E' = 1.5 and U' = 50 x 1.5 = 75 the following comparisons were obtained:

TABLE VII

COMPARISON OF PLANTS C2 AND A2

	WO	DS	AS	HR	MN
C2 ROI (%)	-29.97	49.56	201.04	86.40	28.39
A2 ROI (%)	-32.63	61.60	229.61	61.52	14.06

Again, considering the basic objectives, this was considered close enough to begin an exploration of the surface characteristics of Plant A2.

Plant A2 was first examined only in the valid region with a deterministic direct search technique. Utilizing the relationships prevalent in plant A1, the investigation was conducted such that the progress could be visualized by varying PHI, the recycle split, and FRE, the flow rate of component E out of the reactor, for various values of the other two design variables. It was immediately found that the optimal position for each set of design variables was on the minimum FA feed constraint. Figure 3 shows a representation of this surface when the other design variables were TX = 580°R (temperature in the reactor) and FRC = 1500

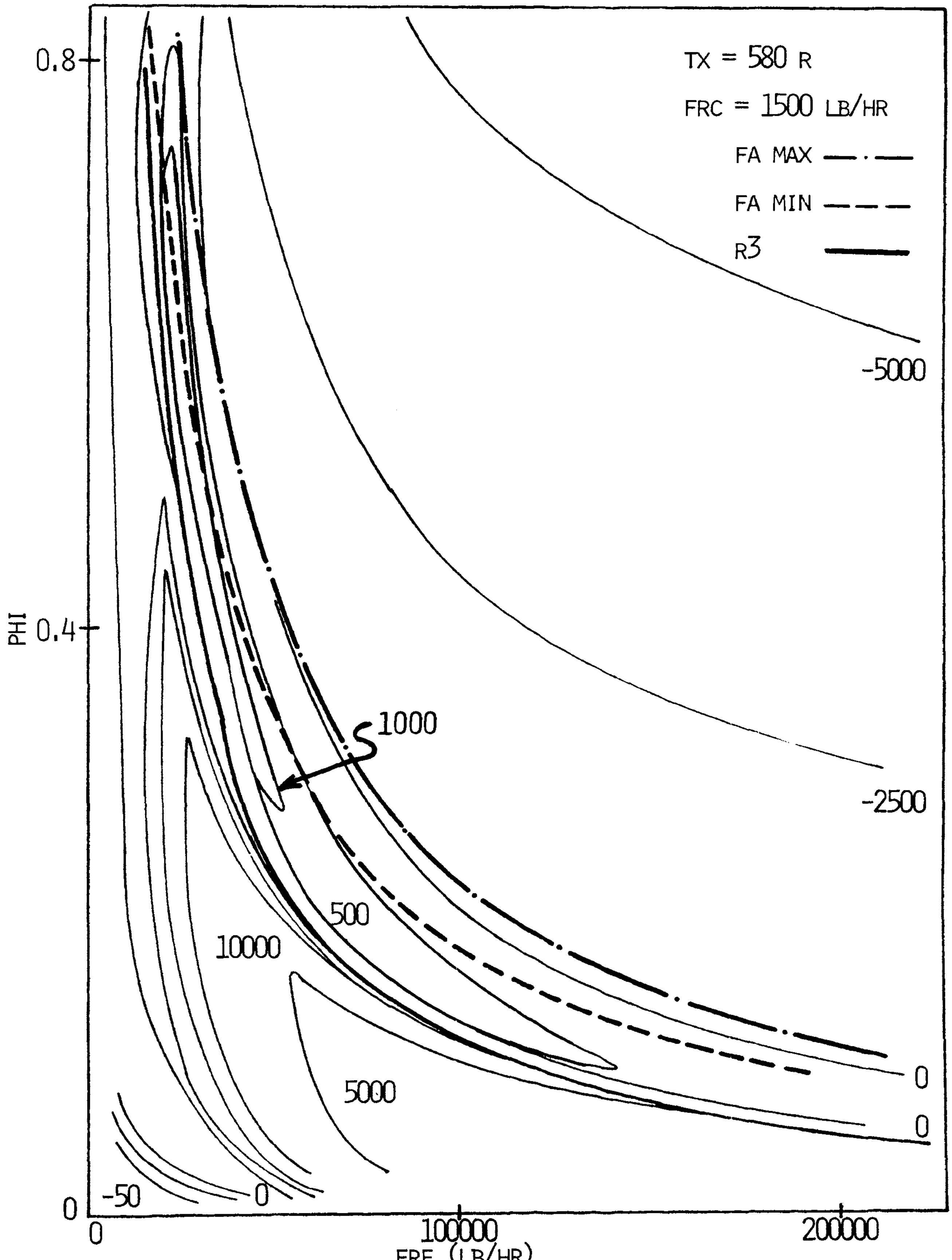


FIGURE 3 CONTOURS OF RETURN ON INVESTMENT - PLANT A2

pounds per hour (flow rate of component C out of the reactor). Concentrating on the parameters for the minimum FA feed constraint, the plant was allowed to reach an optimum value for the four design variables:

TABLE VIII

RETURN ON INVESTMENT CHARACTERISTICS - PLANT A2

FRC = 1000 lb/hr					
TX = 580°R					
PHI	0.90	0.70	0.50	0.30	0.10
ROI (%)	1000	1030	860	570	170
TX = 605°R					
PHI	0.90	0.70	0.50	0.30	0.10
ROI (%)	120	520	590	440	130
TX = 630°R					
PHI	0.90	0.70	0.50	0.30	0.10
ROI (%)	-1000	-50	270	280	80
FRC = 3000 lb/hr					
TX = 580°R					
PHI	0.45	0.35	0.25	0.15	0.05
ROI (%)	840	880	680	370	60
TX = 630°R					
PHI	0.45	0.35	0.25	0.15	0.05
ROI (%)	-1000	0	320	230	30
FRC = 5000 lb/hr					
TX = 580°R					
PHI	0.35	0.25	0.15	0.05	
ROI (%)	0	700	430	80	
TX = 630°R					
PHI	0.35	0.25	0.15	0.05	
ROI (%)	-1000	-200	250	40	

This indicated that the optimal value was against the minimum temperature constraint so more values were examined between FRC values of 1000 and 3000 lb/hr at TX = 580°R. The results are shown in Figure 4 and indicate that the optimum ROI of plant A2, 1000% is at: TX = 580°R, FRC = 1500 lb/hr, PHI = 0.7, and FRE = 22000 lb/hr. The value of the optimum should not be taken literally because of the sensitivity of the economic factors. For example, a change of the total SARE factor to 30% produces an ROI surface that is negative everywhere.

A complete plot of this surface as FRE and PHI vary is the one shown in Figure 3.

Figure 5 shows the return on investment surface of plant A2 at the optimum conditions of plant A1. This shows, graphically, an extrapolation of Table VIII and points out how the A feed constraint intersects the R3 positive definite constraint at lower values of PHI the same as in plant A1, Figure 2. It also shows how the ridge peak generally follows the valid region down to lower values of PHI as the temperature, TX, and flow rate, FRC, are increased.

An additional trial at utilizing a formal optimization technique was attempted on plants A1 and A2. The direct search method of Hooke and Jeeves (19) as modified by Weisman, Wood and Rivlin (35), again with constraints added as suggested by Gottfried, Bruggink and Harwood was used. This method

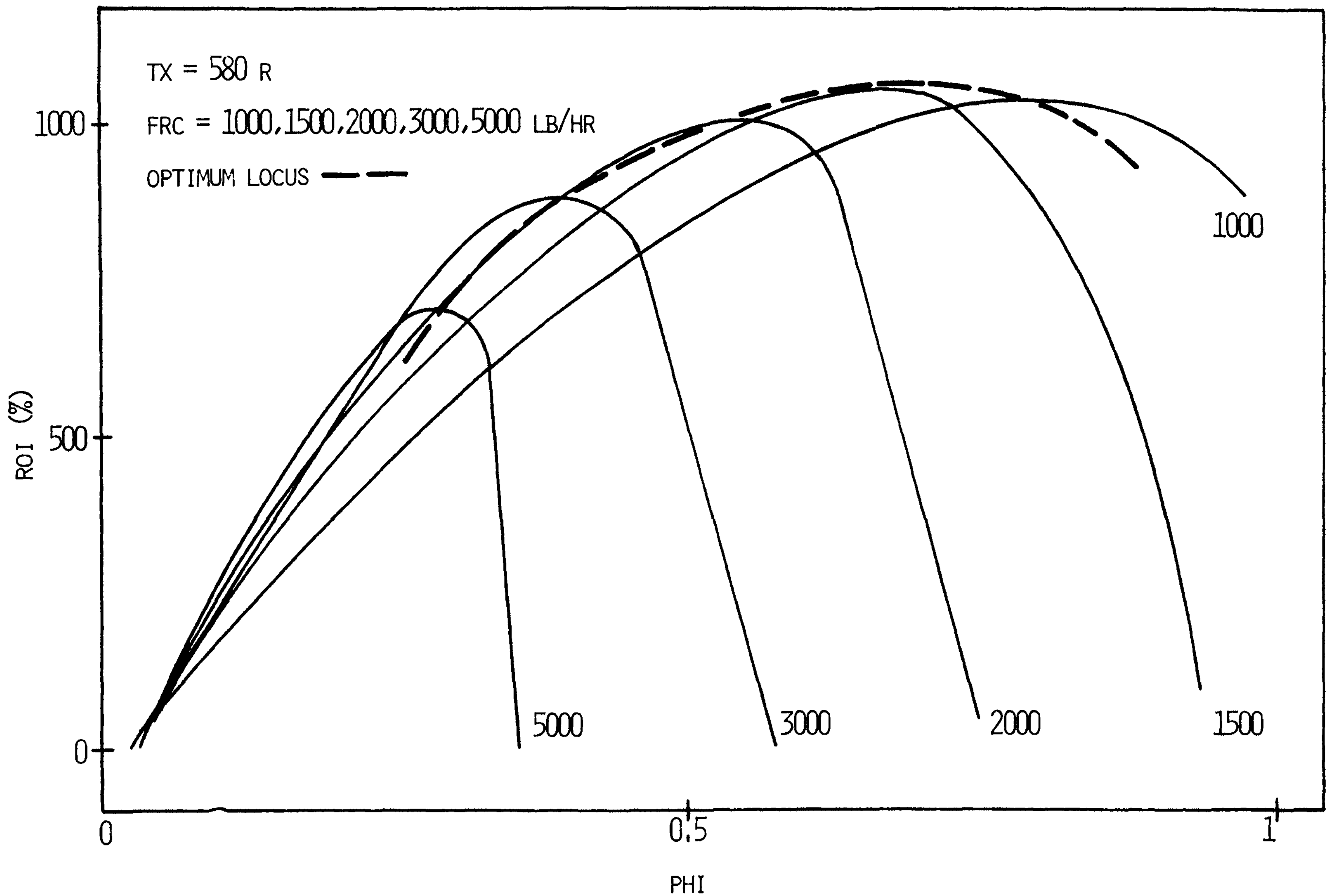


FIGURE 4 PROJECTION OF MINIMUM FEED CONSTRAINT - PLANT A2

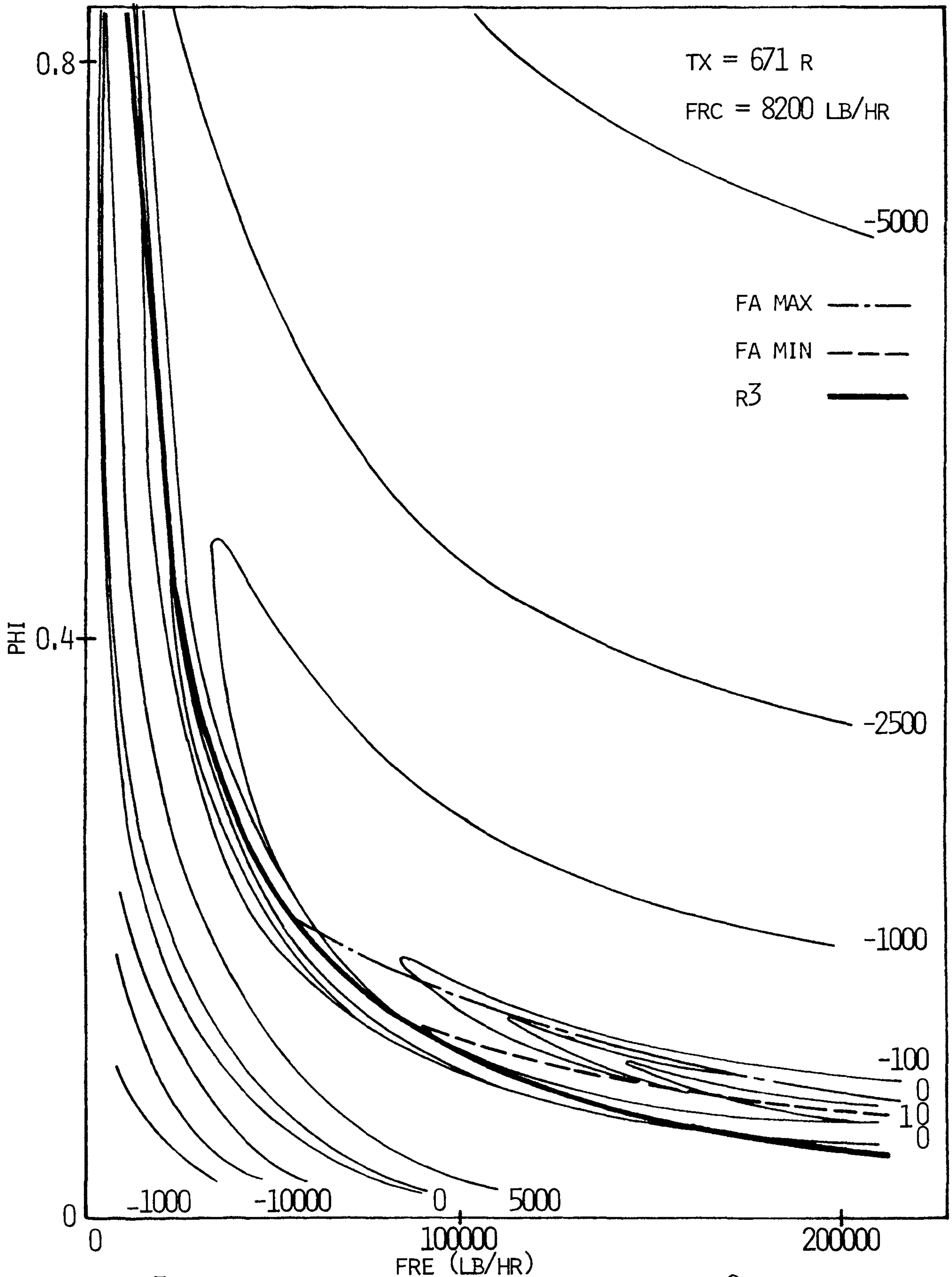


FIGURE 5 CONTOURS OF RETURN ON INVESTMENT - PLANT A2

located the optimum when started from each of the five reported optima mentioned earlier. This approach was more successful than the previous formal optimization techniques probably because of the way it handles the constraints and rotates its steps to follow the curved ridge. The constraints are maintained by the penalty function which is zero inside the valid region and rises as the square of the argument outside. The rate of rise, and the degree of constraint to the valid region, is controlled by a pre-multiplier which is increased until values of the surface within the valid region are maintained. Search times are long, however, and the overall solution effort seems comparable to an intuitive search directed from a computer terminal. Detailed numerical results are presented in Appendix D.

c. Verification

The procedure developed thus far would be useless if the algebraic plant did not yield an optimum near the true optimum. Therefore plant C2 was investigated near the optimum of plant A2. Experiments were run for plant C2 at both 580^{o} and $590^{o}R$ for FRC of 1500, 2000 and 3000 lb/hr:

TABLE IX

RETURN ON INVESTMENT CHARACTERISTICS - PLANT C2

FRC = 1500 lb/hr

PHI	0.65	0.55	0.45	0.40	0.35
(TX = 580^{o}R)ROI(%)	420	425	400	370	340
(TX = 590^{o}R)ROI(%)	360	385	385	375	360

TABLE IX (Cond)

FRC = 2000 lb/hr

PHI	0.65	0.55	0.45	0.40	0.35
(TX = 580°R) ROI(%)	375	445	455	440	420
(TX = 590°R) ROI(%)	175	360	425	430	425

FRC = 3000 lb/hr

PHI	0.50	0.45	0.40	0.35	0.30
(TX = 580°R) ROI(%)	275	440	450	435	400
(TX = 590°R) ROI(%)	-1000	180	420	425	420

Thus, again, the maximum value lies at the minimum temperature constraint and even though the value at 590°R does become greater at lower values of PHI, both values have already reached a peak before this occurs. The results at TX = 580°R are given in Figure 6 and indicate the optimum ROI of plant C2, 450%, is at: TX = 580°R, FRC = 2000 lb/hr, FRE = 34000 lb/hr, PHI = 0.45.

3. Plant Variability

a. Algebraic Examination

In order to understand the reasons for the differences in the optimal operating positions for plant 1 and plant 2, an algebraic examination was appropriate.

Plant 1 was optimized using the objective function proposed by Christensen (5). The general form of this return on investment was:

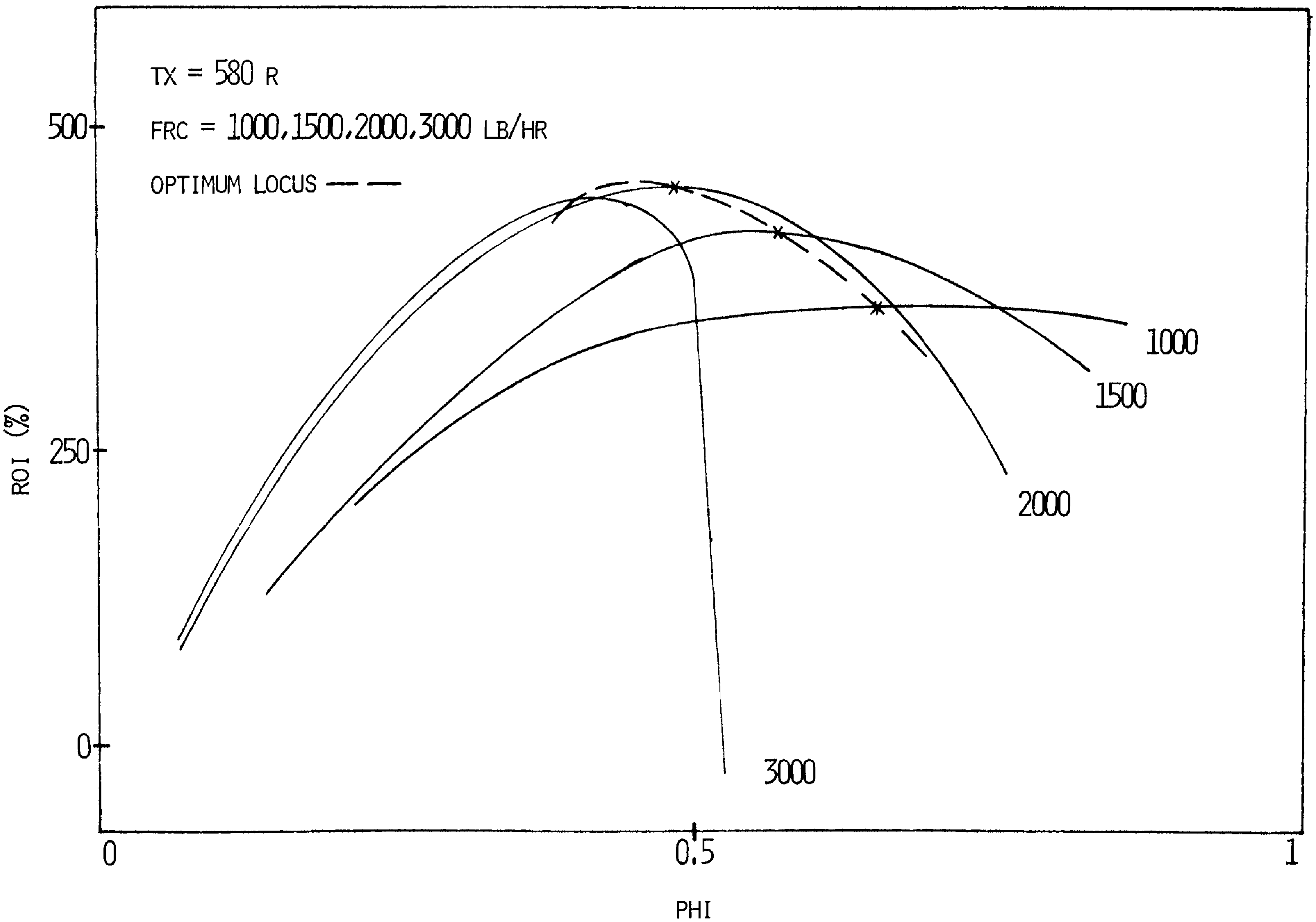


FIGURE 6 PROJECTION OF MINIMUM FEED CONSTRAINT - PLANT C2

$$ROI_1 = \frac{\Sigma gF - 0.37FR}{V\rho} - 10$$

From the algebraic equations (Appendix A) the value of $V\rho$ is determined as follows:

$$V\rho(lb_R) = TAU \cdot FR^2$$

$$TAU(hr^2/lb_R) = R3/k_3FRP \cdot FRC$$

$$R3(lb_C/hr) = (MW_C/MW_P)[R2 - FP - (FRP - FP)PHI]$$

$$R2(lb_B/hr) = (MW_B/MW_E)[FRE \cdot PHI]$$

$$FRP(lb_P/hr) = FP + 0.1FRE$$

Thus:

$$V\rho = \frac{(MW_C/MW_P)[(MW_B/MW_E)FRE \cdot PHI - FP - 0.1FRE \cdot PHI]\ FR^2}{k_3(FP + 0.1FRE)FRC}$$

or:

$$V\rho = b\ FR^2$$

where:

$$b = \frac{2[0.4\ FRE \cdot PHI - FP]}{A_3e^{-B3/T}(FP+0.1FRE)FRC}$$

and the ROI became:

$$ROI_1 = \frac{\Sigma gF}{b\ FR^2} - \frac{0.37}{b\ FR} - 10$$

Plant 2 was optimized using the objective function determined experimentally by CHESS-UMR (14). The general form of this ROI was:

$$ROI_2 = \frac{\Sigma g'F}{E'FR} - \frac{C'}{E'FR} - (CC' + U'/E')$$

Where E' and U' were constants estimated from plant C2 computer output.

The difference between the two ROI's, then was the variability of b and the quadratic FR term in the denominator.

Evaluation of b in terms of FR showed that $b = cFR^{-a}$ where a was greater than 2. Thus

$$ROI_1 = \frac{\Sigma gF - CFR}{cFR^{2-a}} - 10 = \frac{FR^{a-2}}{c} (\Sigma gF - CFR) - 10$$

$$ROI_2 = \frac{\Sigma g'F - C'FR}{E'FR} - KK = \frac{FR^{-1}}{E'} (\Sigma g'F - C'FR) - KK$$

or, in general:

$$ROI_1 \approx FR^{a-2} = \frac{FR^a}{FR^2}$$

$$ROI_2 \approx FR^{-1} = 1/FR$$

Thus, while max ROI_2 occurs at min FR, max ROI_1 depends on the value of a. This basically accounts for the major shift in position of the optimum value because one relation is linear while the other is exponential. The simple linear relation is preferable for this plant, not only for ease of manipulation but also because of a better fit to the investment economics supplied by the simulation routine.

b. Intuitive Examination

The information given for both plants by the response surfaces shown applies equally well to debottlenecking or evolutionary operation because the investment varied so little, roughly 10%, over the entire valid range. This corresponds to the fixed investment characterizing an existing plant which freezes the denominator in the ROI. Thus, the shape of an operating surface is identical with that of the design surface.

The significance of the observation above is that, while a change in the investment correlation procedure very definitely affected the location of the optimum ROI, the overall shape of the objective function remained essentially unchanged. Thus, the objective function selected for this study was actually a function of the revenue or the material balance equations only.

Further examination of the response surfaces for this particular plant, such as those shown in Figures 2, 3, and 5, with additional algebraic and numerical evaluations shows that, although a change in any of the economic factors for SARE, utilities, interest charges - or using total capital as fixed plus working capital - may alter the location of the optimum, the overall shape of the surface remains unchanged. This indicates that the evaluation of any of the response surfaces of the plant will provide sufficient information to choose an appropriate optimization technique. Moreover, the algebraic results for other economic measures such as payout, cash flow, cash flow payout, discounted cash flow, or discounted cash flow payout show that they will have the same general surface shape. This suggests that an investigation into more characteristic or more easily manipulated measures may be worthwhile.

IV. CONCLUSIONS

A. Search programs applicable to chemical plants of the type studied must accept constraints and be able to follow curved ridges.

B. In spite of the apparent complexities of the chemical plants studied, the return on investment response is unimodal within the constraints. Accordingly, intuitive strategies for optimal design would succeed for these plants.

C. The return on investment optimum position is strongly affected by the correlation used for investment for the chemical plants studied.

V. NOMENCLATURE

A	=	Reactant, subscript denotes stream; Arrhenius frequency factor, subscript denotes equation.
A'	=	8400.
ADM	=	Administration cost (CHESS-UMR).
ADVAS	=	Advertising and sales cost (CHESS-UMR).
AMW	=	Molecular weight (CHESS-UMR).
AS	=	Ahlgren & Stevens optimal solution parameters.
A1	=	Algebraic representation of plant 1.
A2	=	Algebraic representation of plant 2.
a	=	Dummy constant.
atm	=	Atmospheres.
B	=	Reactant, subscript denotes stream; Arrhenius activation energy, subscript denotes equation.
B'	=	12600.
BTU	=	British thermal units.
b	=	Dummy variable.
C	=	Intermediate component, subscript denotes stream.
C'	=	5597760.
CC'	=	144/11.
COOL	=	Piping cost (CHESS-UMR)
CSTR	=	Continuous stirred tank reactor.
C1	=	CHESS-UMR representation of plant 1.
C2	=	CHESS-UMR representation of plant 2.
c	=	Dummy constant.
cal	=	Calories.
cm^3	=	Cubic centimeters.

D'	=	2260.9524.
DAYS	=	Operational days per year (CHESS-UMR).
DEP	=	Years to depreciation (CHESS-UMR).
DEP1	=	Salvage value (CHESS-UMR).
DINDX	=	Marshall & Stevens cost index (CHESS-UMR).
DINT	=	Interest cost (CHESS-UMR).
DLBR	=	General labor value (CHESS-UMR).
DMAIN	=	Maintenance cost (CHESS-UMR).
DNCTX	=	Income tax cost (CHESS-UMR).
DNVS	=	Total investment (CHESS-UMR).
DS	=	Dibella & Stevens optimal solution parameters.
d	=	Dummy variable.
E	=	Intermediate component, subscript denotes stream.
E'	=	Experimentally determined constant.
ECONO	=	Research and Development cost (CHESS-UMR).
ECOTSV	=	Value of stream (CHESS-UMR).
EQPAR(23,NE)	=	Utilities cost (CHESS-UMR).
EQPAR(24,NE)	=	Investment cost (CHESS-UMR).
e	=	Base of naperian logarithm.
F	=	Flow rate (pounds per hour), additional letter refers to component or stream.
^{o}F	=	Degrees Fahrenheit.
FR	=	Flow rate out of reactor (pounds per hour), additional letter refers to component.
ft	=	Feet.
ft^2	=	Square feet.
ft^3	=	Cubic feet.

G	=	By product, subscript denotes stream.
G'	=	3324.93.
g,g'	=	Dummy constants.
gal	=	Gallons.
gm mole	=	Gram moles.
H	=	Constraint equation numbered by subscript.
HR	=	Henley & Rosen optimal solution parameters.
hr	=	Hours.
^{o}K	=	Degrees Kelvin.
KWH	=	Kilowatt hours.
k	=	Reaction rate constant, subscript denotes equation.
L/D	=	Reflux ratio in distillation tower.
L/V	=	Liquid-vapor ratio in distillation tower.
lb	=	Pound.
ln	=	Naperian logarithm.
M	=	0.3FP + 0.0068FD - 0.02FA - 0.03FB -0.01FG; one thousand.
MM	=	One million.
MN	=	Mason optimal solution parameters.
MW	=	Molecular weight, subscript denotes component.
m	=	One meter; total number of constraints.
mm	=	One millimeter; with Hg, millimeters mercury.
min	=	Minute.
N	=	Total number of equations.
OC	=	Working capital factor (CHESS-UMR).
OHD	=	Overhead cost (CHESS-UMR).

OTHER	=	Supervision cost (CHESS-UMR).
OTHRS (3)	=	Payroll burden (CHESS-UMR).
OTHRS(4)	=	Labor period (CHESS-UMR).
OTHRS(7)	=	Construction cost factor (CHESS-UMR).
OTHRS(8)	=	Distribution cost (CHESS-UMR).
P	=	Product, subscript denotes stream.
P'	=	99747.9.
PHI	=	Recycle split ratio.
psia	=	Pounds per square inch, absolute.
psig	=	Pounds per square inch, gage.
R	=	Unknown constant in reactor cost equation; reaction mixture; rate of reaction with number.
^oR	=	Degrees Rankine.
ROADS	=	Contingency cost (CHESS-UMR).
ROI	=	Return on investment, subscript denotes plant.
R/R_{min}	=	Ratio of reflux ratio to minimum reflux ratio.
r	=	Unknown constant in reactor cost equation; with subscript, component production rate.
SARE	=	Sales, administration, research, and engineering.
SEXTSV	=	Flow rate (CHESS-UMR).
STM	=	Cost of steam (CHESS-UMR).
SUPP	=	Cost of operating supplies (CHESS-UMR).
sec	=	Seconds.
T	=	Temperature.
TANDI	=	Taxes and insurance cost (CHESS-UMR).
TAU	=	Defined variable ($V\rho/FR^2$).

TELEC	=	Total cost of electricity (CHESS-UMR).
TSTM	=	Total cost of steam (CHESS-UMR).
TTCR	=	Total raw material cost (CHESS-UMR).
TTPC	=	Total sales income (CHESS-UMR).
TWTR	=	Total cost of water (CHESS-UMR).
TX	=	Temperature.
U'	=	Experimentally determined constant.
V	=	Volume.
$V\rho$	=	Pounds of reactor volume.
WO	=	Williams & Otto optimal solution parameters.
WTR	=	Cost of water (CHESS-UMR).
w	=	Dummy function
X	=	Flow rate (pounds per hour) subscript denotes stream; dummy variable.
x	=	Dummy variable.
y	=	Dummy function.
yr	=	Years.
Z	=	Return on investment, dummy function.

GREEK LETTERS AND SYMBOLS

ΔT_{lm}	=	Log-mean temperature difference.
π	=	3.14159···
ρ	=	Density of reaction mixture, 50 pounds per cubic foot.
Σ	=	Summation of elements following.
$	=	Dollars.
%	=	Percent.

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VITA

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APPENDIX A

EXPERIMENTAL APPARATUS - PLANT 1

1. Basic Equation Derivation
2. Algebraic Representation of Plant 1
3. CHESS-UMR Subroutine Description
4. Physical Properties of Components
5. CHESS-UMR Representation of Plant 1

1. Basic Equation Derivation

The equations used for evaluation of all flow rates and the algebraic representation of the return on investment are derived below to better understand the validity of their use.

Defining Equations

Williams and Otto article (38) initially designed the plant.

Reactions taking place in the reactor:

$$A + B \xrightarrow{k_1} C$$

$$C + B \xrightarrow{k_2} P + E$$

$$C + P \xrightarrow{k_3} G$$

where molecular weights are:

$A,B,P = 100$

$C,E = 200$

$G = 300$

Stoichiometry indicates that:

Reaction 1 $\rightarrow$ 2 lbC/lbA and 2 lbC/lbB

Reaction 2 $\rightarrow$ 1 lbP/lbB, 1/2 lbP/lbC, 2 lbE/lbB and 1 lbE/lbC

Reaction 3 $\rightarrow$ 3 lbG/lbP and 3/2 lbG/lbC

Using a subscript to denote the stream containing the component fraction and defining the reaction rate constants as pounds of reaction mixture (R) per pound of A, C, and P per hour respectively, the following rates of component production inside the reactor are obtained:

$$r_A = (-k_1 A_R B_R)V\rho \text{ lbA/hr}$$

$$r_B = (-k_1 A_R B_R - k_2 B_R C_R)V\rho \text{ lbB/hr}$$

$$r_C = (2k_1 A_R B_R - 2k_2 B_R C_R - k_3 P_R C_R)V\rho \text{ lbC/hr}$$

$$r_E = (2k_2 B_R C_R)V\rho \text{ lbE/hr}$$

$$r_P = (k_2 B_R C_R - 0.5k_3 P_R C_R)V\rho \text{ lbP/hr}$$

$$r_G = (1.5k_3 P_R C_R)V\rho \text{ lbG/hr}$$

where $k_i = Ai e^{-(Bi/T)}$ $\quad i = 1,2,3$

TABLE X

ARRHENIUS CONSTANTS

i	Ai $\frac{1}{\text{Hr.wt.fraction}}$	Bi ^{o}R	Basis
1	5.9755×10^{9}	12000	1 pound of A or B
2	2.5962×10^{12}	15000	1 pound of B
3	9.6283×10^{15}	20000	1 pound of C

A mass balance around each piece of mass changing equipment at steady state gives:

Reactor (Assume perfect mixed, constant volume, CSTR where stream FA and FB are pure, and FL contains no component G)

$$0 = FA + FLA_L - FRA_R + (-k_1 A_R B_R)V\rho$$

$$0 = FB + FLB_L - FRB_R + (-k_1 A_R B_R - k_2 B_R C_R)V\rho$$

$$0 = FLC_L - FRC_R + (2k_1 A_R B_R - 2k_2 B_R C_R - k_3 P_R C_R)V\rho$$

$$0 = FLE_L - FRE_R + (2k_2 B_R C_R)V\rho$$

$$0 = FLP_L - FRP_R + (k_2 B_R C_R - 0.5k_3 P_R C_R)V\rho$$

$$0 = -FRG_R + (1.5k_3 P_R C_R)V\rho$$

Decanter (Assume stream FG contains all of the component G in stream FR only)

$$0 = FRA_R - FFA_F$$

$$0 = FRB_R - FFB_F$$

$$0 = FRC_R - FFC_F$$

$$0 = FRE_R - FFE_F$$

$$0 = FRP_R - FFP_F$$

$$0 = FRG_R - FG$$

Distillation tower (Assume FP is pure and there is no component G present)

$$0 = FFA_F - FDA_D - FLA_L$$

$$0 = FFB_F - FDB_D - FLB_L$$

$$0 = FFC_F - FDC_D - FLC_L$$

$$0 = FFE_F - FDE_D - FLE_L$$

$$0 = FFP_F - FDP_D - FLP_L - FP$$

since $FS = FD + FL$ and $FSP_S = FDP_D + FLP_L$ then $P_S = P_D = P_L$. But from Azeotropic characteristics, $P_S = (0.1\ \text{lbP/lbE})(E_S\ \text{lbE/lbS})$, and since FP is pure P, then $E_S = E_F$ and $FP\ E_P = 0$ or $FS\ P_S = 0.1\ FF\ E_F$. The last equation above then becomes:

$$0 = FF\ P_F - 0.1\ FF\ E_F - FP$$

Consolidating by summation gives:

$$FA = FDA_D + (k_1 A_R B_R) V\rho$$

$$FB = FDB_D + (k_1 A_R B_R + k_2 B_R C_R) V\rho$$

$$0 = FDC_D - (2k_1 A_R B_R - 2k_2 B_R C_R - k_3 P_R C_R) V\rho$$

$$0 = FDE_D - (2k_2 B_R C_R) V\rho$$

$$FP = FDP_D + (k_2 B_R C_R - 0.5k_3 P_R C_R) V\rho$$

$FG = (1.5k_3P_RC_R)V\rho$

$FR = FRA_R + FRB_R + FRC_R + FRE_R + FRP_R + FRG_R$

$FP = FFP_F - 0.1FFE_F$

Dibella and Stevens (8) were able to simplify the system considerably by noticing several recurrent combinations throughout the equations as written. In the first five equations, as previously defined, all contain the form FDX_D (where X_D is lbX/hr in stream D). But X_D = X_R/FS (where FS = FR - FG - FP) and thus $FDX_D = X_R(FD/FS)$.

The first six equations as previously defined, all contain the forms $k_1A_RB_R$, $k_2B_RC_R$ and $k_3P_RC_R$. Combining this form with the X_R form above, a new variable was defined of the form FRX = lbX/hr, and the equations may be written:

$$FA = FRA(FD/FS) + \left[k_1\left(\frac{FRA\cdot FRB}{FR^2}\right)\left(\frac{MW_A}{MW_B}\right)\right] V\rho$$

$$FB = FRB(FD/FS) + \left[k_1\left(\frac{FRA\cdot FRB}{FR^2}\right) + k_2\left(\frac{FRB\cdot FRC}{FR^2}\right)\right] V\rho$$

$$0 = FRC(FD/FS) - \left[k_1\left(\frac{FRA\cdot FRB}{FR^2}\right)\left(\frac{MW_C}{MW_B}\right) - k_2\left(\frac{FRB\cdot FRC}{FR^2}\right)\left(\frac{MW_C}{MW_B}\right) - k_3\left(\frac{FRP\cdot FRC}{FR^2}\right)\right] V\rho$$

$$0 = FRE(FD/FS) - \left[k_2\left(\frac{FRB\cdot FRC}{FR^2}\right)\left(\frac{MW_E}{MW_B}\right)\right] V\rho$$

$$FP = -FRP(FD/FS) + \left[k_2\left(\frac{FRB\cdot FRC}{FR^2}\right)\left(\frac{MW_P}{MW_B}\right) - k_3\left(\frac{FRP\cdot FRC}{FR^2}\right)\left(\frac{MW_P}{MW_C}\right)\right] V\rho$$

$$FG = \left[k_3\left(\frac{FRP\cdot FRC}{FR^2}\right)\left(\frac{MW_G}{MW_C}\right)\right] V\rho$$

$$FR = FRA + FRB + FRC + FRE + FRP + FG$$

$$FP = FRP - 0.1FRE$$

Christensen (5) took the equations defined by Dibella and Stevens and again simplified the system by defining five new variables.

Define:

$$PHI = (FD/FS) = FD/(FR - FG - FP)$$

$$TAU = V\rho/FR^2$$

$$R1 = k_1 \frac{FRA \cdot FRB \cdot V\rho}{FR^2} = A_1 e^{-B_1/T}\ FRA \cdot FRB \cdot TAU$$

$$R2 = k_2 \frac{FRB \cdot FRC \cdot V\rho}{FR^2} = A_2 e^{-B_2/T}\ FRB \cdot FRC \cdot TAU$$

$$R3 = k_3 \frac{FRP \cdot FRC \cdot V\rho}{FR^2} = A_3 e^{-B_3/T}\ FRP \cdot FRC \cdot TAU$$

and the six previously defined equations become:

$$FA = R1 + FRA \cdot PHI$$

$$FB = R1 + R2 + FRB \cdot PHI$$

$$FRC = (1/PHI)\left[\left(\frac{MW_C}{MW_B}\right)(R1 - R2) - R3\right]$$

$$FRE = (1/PHI)\left[\left(\frac{MW_E}{MW_B}\right) R2\right]$$

$$FP = R2 - \left(\frac{MW_P}{MW_C}\right) R3 - (FRP - FP)\ PHI$$

$$FG = \left(\frac{MW_G}{MW_C}\right) R3$$

$$FR = FRA + FRB + FRC + FRE + FRP + FG$$

$$FP = FRP - 0.1FRE$$

So there are there are thirteen equations in seventeen variables for a given FP: FA, FB, FRA, FRB, FRC, FRE, FRP, FD, FG, FR, PHI, R1, R2, R3, T, TAU, and V.

The best method of solution for these thirteen equations was determined by Christensen's algorithm II-T (5) to be to first specify T, PHI, FRE and FRC as the design variables, then solve equations in the following order:

$$FRP = FP + 0.1FRE$$

$$R2 = \left(\frac{MW_B}{MW_E}\right)(FRE \cdot PHI)$$

$$R3 = \left(\frac{MW_C}{MW_P}\right)(R2 - FP - FRP \cdot PHI - FP \cdot PHI)$$

$$R1 = \left(\frac{MW_B}{MW_C}\right)(R3 + FRC \cdot PHI) + R2$$

$$k_i = A_i e^{-(B_i/T)}, \quad i = 1,2,3$$

$$TAU = R3/(k_3 \cdot FRP \cdot FRC)$$

$$FRB = R2/(k_2 \cdot FRC \cdot TAU)$$

$$FRA = R1/(k_1 \cdot FRB \cdot TAU)$$

$$FB = R1 + R2 + FRB \cdot PHI$$

$$FG = \left(\frac{MW_G}{MW_C}\right) R3$$

$$FR = FRA + FRB + FRC + FRE + FRP + FG$$

$$FD = PHI(FR - FG - FP)$$

$$FA = R1 + FRA \cdot PHI$$

$$V = TAU \cdot FR^2/\rho$$

Return on Investment

The ROI was initially defined by Williams and Otto as:

$$ROI = \frac{100[8400(M) - 2.22FR - (0.124)(8400)(0.3FP + 0.0068FD) - 276000]}{2780000}$$

where 8400 = hr/yr

$$M = 0.3FP + 0.0068FD - 0.02FA - 0.03FB - 0.01FG$$

$0.3FP + 0.0068FD$ = product sales, \$/hr

$- 0.02FA - 0.03FB$ = raw material cost, \$/hr

$- 0.01FG$ = waste disposal cost, \$/hr

$2.22FR$ = utilities charges, \$/yr

$(0.124)(8400)(0.3FP + 0.0068FD)$ = SARE expenses, \$/yr

276000 = plant fixed charges consisting of depreciation, factory indirect expense, labor, supervision, payroll charges, repairs and laboratory expenses, \$/yr

2780000 = total investment consisting of fixed plus working capital.

At the suggestion of Williams and Otto, Dibella and Stevens set the fixed charges and investment proportional to the optimal value for $V\rho$ reported by Williams and Otto of 4640 pounds. Thus:

$$276000 = a_1 V\rho \Longrightarrow a_1 \approx 60$$

$$2780000 = a_2 V\rho \Longrightarrow a_2 \approx 600$$

and the equation becomes:

$$z = \frac{100[8400(M) - 2.22FR - (0.124)(8400)(0.3FP + 0.0068FD) - 60\ V\rho]}{600V\rho}$$

Christensen collected terms and developed the objective function used in the present study for plant A1:

$$z = \frac{(368FP + 8.4FD - 28FA - 42FB - 14FG - 0.37FR)}{V\rho} - 10$$

Constraints indicated by Christensen are applicable:

$$580 \leq T \leq 680$$

$$12400 < FA < 16600$$

$$0 < PHI < 1$$

$$0 < R3$$

and should be checked as soon as possible in the solution procedure.

2. Algebraic Representation of Plant 1

In order to establish a base from which to work, Williams and Otto's optimal solution was considered as the most significant set of values. Following is a plant design based on the optimal values reported by Williams and Otto:

Flow Rates

TABLE XI

MASS BALANCE AT WILLIAMS AND OTTO OPTIMUM

Stream	A	B	C	E	P	G	Total
FA lb/hr	14502	0	0	0	0	0	14502
Fraction	1.0000						1.0000
FB lb/hr	0	33325	0	0	0	0	33325
Fraction		1.0000					1.0000
FR lb/hr	11623	36777	2351	33348	8098	3719	95916
Fraction	0.1212	0.3834	0.0245	0.3477	0.0844	0.0388	1.0000
FG lb/hr	0	0	0	0	0	3719	3719
Fraction						1.0000	1.0000
FF lb/hr	11623	36777	2351	33348	8098	0	92197
Fraction	0.1261	0.3989	0.0255	0.3617	0.0878		1.0000
FP lb/hr	0	0	0	0	4763	0	4763
Fraction					1.0000		1.0000
FS lb/hr	11623	36777	2351	33348	3335	0	87434
Fraction	0.1329	0.4206	0.0269	0.3814	0.0381		1.0000
FD lb/hr	5230	16550	1058	15007	1501	0	39346
Fraction	0.1329	0.4206	0.0269	0.3814	0.0381		1.0000
FL lb/hr	6393	20227	1293	18341	1834	0	48088
Fraction	0.1329	0.4206	0.0269	0.3814	0.0381		1.0000

From this mass balance it is apparent that there is:

1058 lbC produced per hour

15007 lbE produced per hour

6264 lbP produced per hour

3719 lbG produced per hour

EQUIPMENT

Reactor

The volume of the reactor was determined from the algebraic equations to be 92.8 ft^3. From Figure 2 in the Williams and Otto article the vapor pressure must be approximately 2500 mm Hg at 640°R to maintain a liquid reaction. The heats of reaction given in the original article (38) produce the following total heat of reaction:

Equation 1 (-125 BTU/lbC)(1058 lbC/hr)	= - 132 200 BTU/hr
Equation 2 (-50 BTU/lb(E+P))(15007 lbE/hr + 6264 lbP/hr)	= -1 063 000 BTU/hr
Equation 3 (-143 BTU/lbG)(3719 lbG/hr)	= - 532 000 BTU/hr
Total	= -1 727 200 BTU/hr

The heat required to bring the reactants up to the reaction temperature is:

(14502 lb/hr)(0.4 BTU/lb°F)(180 - 70)°F	= 637 500 BTU/hr
(33325 lb/hr)(0.4 BTU/lb°F)(180 - 70)°F	= 1 467 000 BTU/hr
(48088 lb/hr)(0.4 BTU/lb°F)(180 - 100)°F	= 1 540 000 BTU/hr
Total	3 644 500 BTU/hr

It is obvious that approximately 2 mm BTU/hr must be added to the reactor in order to maintain the desired temperature. This does not correspond with Williams and Otto who indicate a necessity for cooling the reactor.

Heat Exchanger

The cooling water varies from 60^oF to 80^oF and the reactant must vary from 180^oF to 100^oF.

Heat = (95915 lb/hr)(0.4 BTU/lb^{o}F)(100 - 180) = -3 070 000 BTU/hr

Cooling Water = (3070000 BTU/hr)/(1 BTU.lb^{o}F)(80 - 60) = 153 500 lb/hr

Area = (3070000 BTU/hr)/(82.5 BTU/hr ft^{2o}F)(ΔT_{lm}) = 569 ft^2

Decanter

Volume flow rate through the decanter is: (95915 lb/hr)/(50 lb/ft^3) = 1918 ft^3/hr. Assuming a 5.8 minute residence time the decanter volume is: (1918 ft^3/hr)(5.8 min)/(60 min/hr) = 185 ft^3.

Distillation Column

Assume binary separation, liquid feed, equimolar overflow and a total condenser. A McCabe-Thiele (26) plot indicates that fourteen theoretical plates are required for the desired separation. This indicates that the original article considered plate efficiencies of approximately 70%. The feed plate is the third theoretical plate from the bottom. Calculations also indicate:

L/D = 87433/4763 = 18.4

L/V = 87433/92196 = 0.958

L/V (minimum) = 0.92 from McCabe-Thiele plot

$R/R_{minimum}$ = 0.958/0.92 = 1.04

The feed enters the column at 100°F as saturated liquid so the feed plate pressure must be 330 mm Hg. Assuming a pressure drop of 4 mm Hg per tray, the pressure into the condenser is 270 mm Hg corresponding to saturated vapor at 94°F. Assuming a vapor density of 0.0725 lb/ft^3 the vapor velocity is:

$$(92196 \text{ lb/hr})\left(\frac{4}{100\,\pi \text{ ft}^2}\right)\left(\frac{1}{0.0725 \text{ lb/ft}^3}\right)\left(\frac{1}{3600 \text{ sec/hr}}\right) = 4.5 \text{ ft/sec}$$

<u>Condenser</u>

Assume a pressure drop of 28 mm Hg in the condenser, the temperature out must be 89°F. Thus the condenser must both condense and cool. Assume a 25°F change in cooling water.

Heat = (92196 lb/hr)(-95 BTU/lb + 0.4 BTU/lb°F(89 - 94)) = -8950000 BTU/hr

Cooling water = (8950000 BTU/hr)/(1 BTU/lb°F)(25°F) = 358000 lb/hr

Area = (8950000 BTU/hr)/(150 BTU/hr ft^2°F)(ΔT_{1m}) = 4300 ft^2

<u>Accumulator</u>

Assume a six minute residence time.

(92196 lb/hr)(0.1 hr)(7.48 gal/ft^3)/(50 lb/ft^3) = 1380 gal

<u>Reboiler</u>

Assume 20% of the boilup is vapor and, considering equimolar overflow, the reboiler feed must be (92196 lb/hr)/(0.2) = 462000 lb/hr at 350 mm Hg and 121°F. Since the bottoms stream is withdrawn before reboiler feed, however, the total mass flow out the bottom of the tower is 549433 lb/hr.

Heat = (462000 lb/hr)(0.2)(95 BTU/lb) = 8770000 BTU/hr

Hot water = (8770000 BTU/hr)/(1 BTU/lb°F)(150 - 130) = 438000 lb/hr

Area = (8770000 BTU/hr)/(700 BTU/hr ft^2°F)(ΔT_{1m}) = 500 ft^2

Sump

Assume a six minute residence time.

(549433 lb/hr)(0.1 hr)(7.48 gal/ft^3)/(50 lb/ft^3) = 8220 gal

MISCELLANEOUS EQUIPMENT

Williams and Otto's remaining equipment is not designated in sufficient detail to warrant an attempt at correlation.

ECONOMICS

An estimate of individual equipment costs is based on the cost curves in Peters and Timmerhaus (29). A conversion factor of 0.919 was used to account for the change in the Marshall and Stevens Index (33) from 1959 to 1967.

Reactor 92.8 ft^3 = 695 gal at 44 psi fig 13.56 (200 psig, carbon steel)	\$ 3220
Decanter 185 ft^3 = 1385 gal at 1 atm fig 13.56 (storage tank, steel)	\$ 1380
Accumulator 1380 gal fig 13.56 (storage tank, steel)	\$ 1380
Sump 8220 gal fig 13.56 (storage tank, steel)	\$ 3580
Tower 10 ft diameter, 20 trays fig 15.21 (bubble trays, steel)	\$30000
Heat Exchanger 569 ft^2 fig 14.15 (150 psi, 300^{o}F, bare steel)	\$ 3220
Condenser 4260 ft^2 fig 14.15 (150 psi, 300^{o}F, bare steel)	\$13800
Reboiler 500 ft^2 fig 14.15 (150 psi, 300^{o}F, bare steel)	\$ 3030
Total	\$59610

This total equipment cost is so far from the \$382,000 indicated by Williams and Otto that an undeterminable, radical difference in design policy must be assumed for the Williams and Otto article. The \$382,000 value was used for the remainder of the calculations for plant 1, however, in order to determine the reasoning behind the selection of various expenses reported. Following is an analysis of Appendices VII and VIII and Figure 19 of Williams and Otto's article:

TABLE XII

ECONOMIC ANALYSIS OF PLANT 1

EXPENSES

I. Total Manufacturing Capital = \$1,035,000

This is normally the total process equipment cost times a Lang factor (24). If the \$382,000 figure reported is used, the Lang factor is 2.71 which is low. If the \$60,000 figure calculated here is used, the Lang factor is 17 which is too high. It was impossible to accurately verify the \$1,035,000 figure, therefore, but \$1,035,000 was used to correlate the remaining economics.

A. Raw materials = 10,836,000 \$/yr

(121800 m lbA/yr)(20 \$/m lbA) = 2,436,000 \$/yr

(280000 m lbB/yr)(30 \$/m lbB) = 8,400,000 \$/yr

These values are equivalent to the (14500 lbA/hr)(0.02 \$/lbA) and (33350 lbB/hr)(0.03 \$/lbB) feeds.

B. Direct expense = 690,000 \$/yr

1. Utilities = 212,300 \$/yr

a. Steam = (84000 m lb/yr)(1.00 \$/m lb) = 84000 \$/yr

This is equivalent to the capacity production of 10000 lb/hr at 0.001\$/lb.

b. Water = (500000 m gal/yr)(0.25 \$/m gal) = 125,000 \$/yr

According to Williams & Otto's calculations there is a total requirement for 519900 lb H_2O/yr including 10400 lb/hr in the reactor. The water cost given above is equivalent to 519900 lb/hr at 0.00025 \$/gal.

c. Electricity = (330000 KWH/yr)(0.01 \$/KWH) = 3300 \$/yr

There is no way to accurately estimate the procedure used by Williams and Otto to determine this value, but in comparison to the other values under consideration, the figure is insignificant.

2. Waste Disposal

(3714.2 lbG/hr)(0.01 \$/lbG)(8400 hr/yr) = 311700 \$/yr

3. Salaries = 166000 \$/yr

a. Supervision = 10,000 \$/yr

There is a requirement for one part time supervisor so he must receive 10,000 \$/yr.

b. Labor = 50,000 \$/yr

There is a requirement for two laborers who must be paid at the rate of 5.80 \$/hr.

c. Payroll charges = 6,000 \$/yr

This is 10% of the 60,000 \$/yr labor and supervision charges.

d. Repairs = 50,000 \$/yr

This is 4.85% of the \$1,035,000 manufacturing capital.

e. Laboratory = 50,000 \$/yr

This is 4.85% of the \$1,035,000 manufacturing capital and includes the chemist salary.

II. Total Direct Manufacturing Cost = 11,526,000 \$/yr

This is the sum of raw material cost and direct expense.

III. Indirect Expense or Cost = 110,000 \$/yr

A. Depreciation = 104,000 \$/yr

This is 10% of the \$1,035,000 manufacturing capital.

B. Factory Indirect Expense = 6,000 \$/yr

This is 0.58% of the \$1,035,000 manufacturing capital.

IV. Total Conversion = 800,000 \$/yr

This is the sum of the direct and indirect expense.

V. Total Manufacturing Cost = 11,636,000 \$/yr

This is the sum of the direct and indirect costs.

ESTIMATE OF CAPITAL REQUIREMENTS

I. Manufacturing Capital	
Total Process Equipment	\$ 382 000
Total Manufacturing Capital, Lang Factor 2.71	\$1 035 000
Contingency at 0%	\$ 0
Total Manufacturing Cost Estimate	\$1 035 000
II. Nonmanufacturing Capital	
31% of Manufacturing Capital	\$ 321 000
III. Total Fixed Capital	
Sum of I and II	\$1 356 000
IV. Working Capital	
10% of Gross Sales	\$1 424 000
V. Total Fixed and Working Capital	
Sum of III and IV	\$2 780 000

ESTIMATE OF ANNUAL EARNINGS AND RETURN

I.	Gross Sales	
	Production Rate lb/yr	8400 hr/yr(4763 lbP/hr + 39376 lbD/hr)
	Sales Price $/lb	0.30 $/lbP and 0.0068 $/lbD
	Gross Sales Income	14,240,000 $/yr
II.	Less Manufacturing Costs	
	Manufacturing Costs	11,636,000 $/yr
	Gross Profit	2,604,000 $/yr
III.	Less SARE	
	SARE Expenses at 12.4% of Sales	1,769,000 $/yr
	Net Income Before Tax	835,000 $/yr
IV.	Less Income Tax	
	Income Tax at 0%	0
	Net Annual Earnings	835,000 $/yr
V.	Return on Total Investment	
	Net annual earnings	835,000 $/yr
	Total Fixed and Working Capital	2,780,000 $
	% Net Return	30.1 %

3. CHESS-UMR Subroutine Description

In order to obtain a realistic model of the chemical plant, CHESS-UMR (14) was used.

For this plant, the entire return on investment surface is adequately described by mass balances. Christensen (5) pointed out perhaps the simplest system of fourteen equations in eighteen variables. Using the four design variables recommended by Christensen's algorithm II-T, the complete plant flow rates can be solved without iteration. For any optimization procedure, the objective function must necessarily be evaluated several times so that it should be obtained by the simplest, quickest and most direct route for efficient optimization.

CHESS-UMR was used therefore only to evaluate the equipment size and costs, with all flowrates calculated prior to entry into any of the specific equipment calculations. With both CHESS-UMR and the design equations, a model of the chemical plant was obtained which possessed both realism and ease of solution.

The model used in CHESS-UMR is shown in Figure 7. The variations from the original plant were only for manipulation. The subroutines used in CHESS-UMR are described below.

DUMEQP - This subroutine is provided in CHESS-UMR to allow for items of equipment not included in the program to be calculated and considered in the plant system. It is accessed through nineteen entry points called ADD1 through AD19.

ADD1 - is the main calculational subprogram in the plant. This subprogram receives the four design variables: FRC, FRE, TX, and PHI plus the operating pressure and the ratio of the reflux ratio

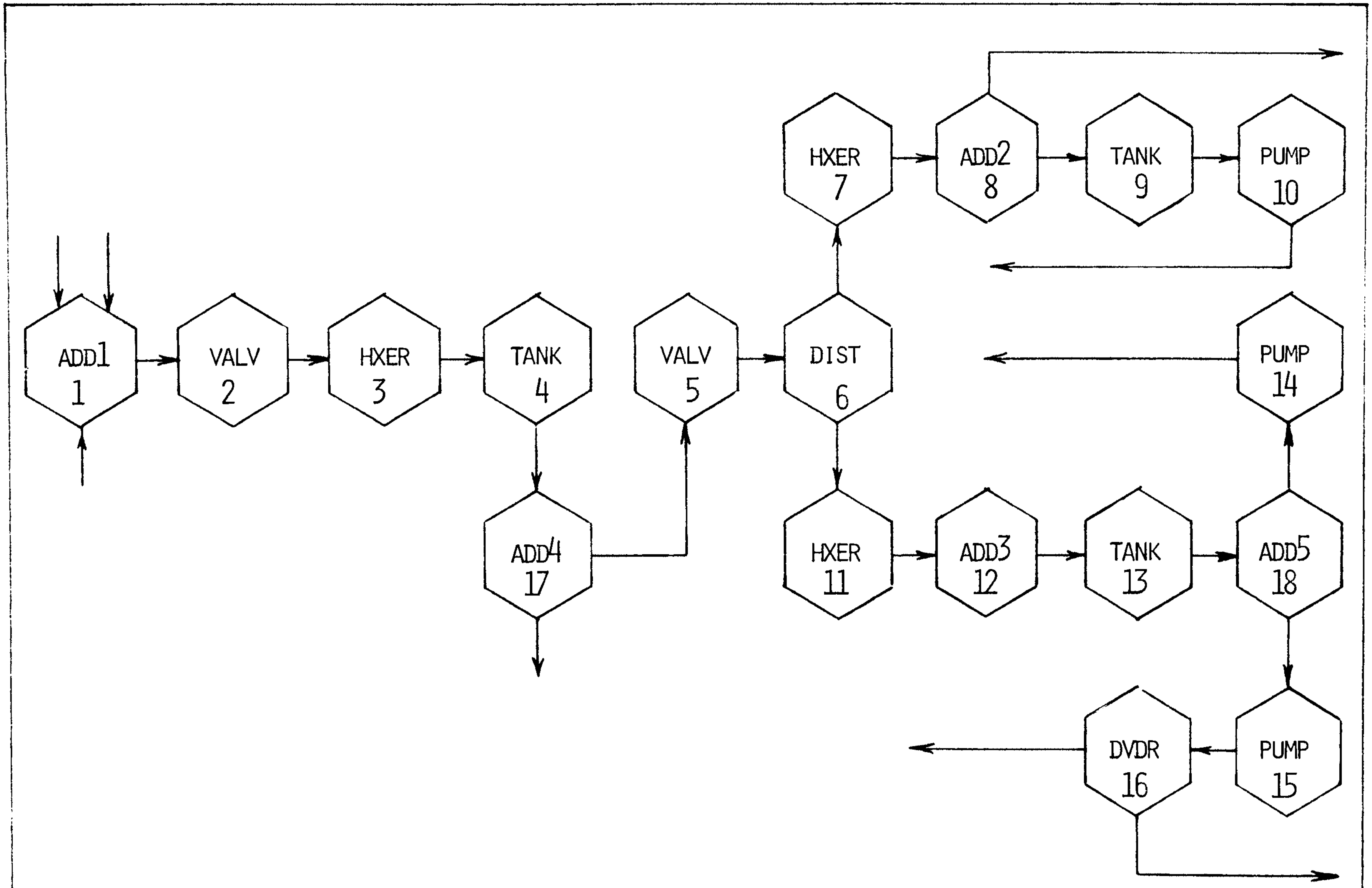

FIGURE 7 CHESS-UMR CHEMICAL PLANT

to the minimum reflux ratio in the distillation tower. ADD1 first calculates the pressure in the reactor based on the vapor pressure given in Williams and Otto's article. The equation used delivers the pressure in mm Hg with temperature given in ^{o}F so the pressure must be converted to psia and psig to be used in later calculations by CHESS-UMR. Pressure of the input streams to the reactor are set equal to the pressure calculated at the given temperature. ADD1 then calculates every plant flow rate and the reactor volume from the thirteen independent equations. In order to estimate the heating or cooling required for reaction, the heats of reaction are calculated and totaled from the heats of reaction given by Williams and Otto. The heat required to bring the reacting materials to the reaction temperature is then calculated using the simple specific heat relationship (Smith and Van Ness (32)). The difference between these two energy values is the amount of heat required to be transfered for the isothermal reactor. The utilities cost is then calculated, for heating based on condensing steam at atmospheric pressure and for cooling based on the same source of cooling water used in the reaction heat exchanger. The cost of the reactor is calculated next using the data of Figure 13-89 in Peters and Timmerhaus (29). The costs are broken down into three curves based on the pressure in the steel reactor (50,300 and 1500 psig). The equations were calculated from the relationship: $\$ = R(V)^r$ or $\ln\$ = \ln R + r\ln V$. The points chosen for evaluation and constants determined were: 50 psig - 100 &

1000 gal and 2600 & 8900 $ giving 235 for R and 0.535 for r; 300 psig - 100 & 500 gal and 3400 & 8000 $ giving 295 for R and 0.530 for r; 1500 psig - 100 & 300 gal and 23000 & 40000 $ giving 2250 for R and 0.503 for r. These equations deliver the investment cost in 1967 dollars with volume given in gallons. After these calculations are made, all flow rates are converted from pounds per hour to pound mole per hour for use in CHESS-UMR. The remainder of this subprogram establishes the parameters for use throughout the program to minimize the necessity of reading in several cards of data when only one item is changed. First, the temperature, pressure and composition of all reactor input and output streams are established as calculated by the mass balance. Then the recycle stream is set equal to the third input stream to the reactor in order to establish the recycle loop without having CHESS-UMR do any recycle calculations. The distillation tower pressure and ratio of reflux ratio to minimum reflux ratio are established as those read into this subprogram. The actual fraction of the product P coming out of the reactor that is to be the overhead product is then established for use by the distillation tower. The pressure produced by the reflux pump is set at 15 psia over the distillation tower pressure to allow for distribution of the overhead product. The pressure produced by the tower bottom pump is set at 2.15 psia over the column pressure to allow for pressure drop through the reboiler. The recycle pump outlet pressure is set equal to the reactor pressure. Finally the recycle split to be used by the divider is established as the input, PHI.

ADD2 and ADD3 - are added to the chemical plant in order to allow for economic evaluation of the reflux and recycle accessories respectively. Both subprograms assume equimolar overflow. Since the tower is designed to operate with a total condenser in CHESS-UMR, the reflux pump and accumulator must be capable of handling the entire mass flow rate out the top of the tower. The total mass flow out the bottom of the column is the bottom product plus the vapor flow rate. In ADD2 the product stream is added to the vapor flow rate to arrive at the true total flow rate out the top of the tower. In ADD3 the tower bottom flow rate is calculated.

ADD4 - is added to the chemical plant in order to separate the waste material G from the reactor products. The entire subprogram consists of simply setting the physical properties to the two output streams.

ADD5 - is added to the chemical plant in order to separate the tower bottom product from the vapor reflux flow. CHESS-UMR calculates the reboiler by assuming that the tower bottom product is separated prior to entry into the reboiler, then the entire flowrate into the reboiler is vaporized.

VALV - This subroutine in CHESS-UMR allows for a decrease in flowstream pressure. It computes the temperature and vapor fraction of the output stream at the enthalpy of the input stream and the specified output stream pressure. The diameter of the valve is taken as pipe diameter which is computed using an average liquid velocity of four feet per second and a vapor velocity of ten feet per second.

HXER - This subroutine provides heating or cooling of a flow stream. The output temperature is computed along with the heat transfer area based on the heat duty calculations with water or steam as the source of cooling or heating. The overall heat transfer coefficient, number of shells, number of tube and shell passes per shell, type of exchanger, pressure drop on both the tube and shell sides, and construction materials are specified for all types of heat exchangers. The cooling water temperature may be specified for both inlet and outlet conditions or they will be set by CHESS-UMR at 550^{o} & $565^{o}R$ respectively. For the reaction heat exchanger, the output temperature is specified and only the area and heat duty are calculated. For the reboiler, the steam pressure is specified as 150 psia. The subroutine returns all temperatures, heat duty, area, investment, utilities costs, and the mass of heating or cooling fluid required.

TANK - This subroutine provides the size and investment required for a holding tank based on the holdup time as specified. The physical properties of the stream are obtained by CHESS-UMR from other parts of the program.

DIST - This subroutine designs the distillation tower. Input to the subroutine is the designation of the light and heavy key, ratio of reflux ratio to minimum reflux ratio, type of trays, fraction of each component in the feed to be in the overhead product, and material of construction. The program calculates the number of trays by the Fenske-Underwood-Gilliland method. The tray spacing is based on the diameter with 18 inch spacing for diameters less than 4 feet and 24 inch spacing for 4 foot diameters and greater. The subroutine is used in conjunction with two heat exchangers specifically designated as condenser and reboiler. These exchangers take the fraction of the column feed as their output products and use the reflux ratio calculated in DIST to determine their area and heat duty, the combination of these three subroutines calculates the distillation tower, the condenser, and the reboiler. The condenser output is the overhead product and reflux is considered internally. The reboiler output is the bottom product and the vapor reflux is considered internally. The combination of subroutines as written, therefore, does not allow for economic evaluation of either condenser or reboiler reflux pumps and tanks. Since these items were to be included in the economic evaluation of the plant, the ADD2 and ADD3 subprograms were written and incorporated in the overall program.

PUMP - This subroutine provides an increase in pressure of a flowing stream. Input to the subroutine is an estimate of the work capacity in BTU per hour, output pressure in psia, type of motive power, number of pumps in parallel, whether centrifugal or reciprocating type, number of spare pumps, and material of construction.

The program calculates the size based on the flowrate and pressure rise after correcting for temperature and suction pressure.

DVDR - This subroutine provides a simple split of a flow stream. Input to the subroutine is the fraction of the input stream to be allocated to each output stream.

The other primary contributing subroutine utilized by CHESS-UMR in the plant simulations is the economic subroutine, ECON. This subroutine was written at the University of Missouri-Rolla and consists of two basic subdivisions.

Investment summary starts with the sum of the basic equipment costs and adds a factor to account for process piping, to arrive at a total installed plant cost. This total installed plant cost is increased by 21.4% to account for site development and facilities. The new total installed plant cost is modified by a variable factor to account for geographic location and then the contingency is added to arrive at the total investment completing the investment summary.

Economic data is divided into twelve different sections.

Working capital is computed as 5% of the total investment plus a variable percentage of the sales.

Revenue is simply calculated as the product flow rates times the selling price. Waste products are also considered here with negative prices.

Variable costs include the total utilities costs calculated by each equipment subroutine, and the operating supplies calculated as a variable percentage of the labor.

Fixed costs consist of variable factors for labor, supervision, payroll burden, overhead, maintenance, taxes and insurance, depreciation, and interest.

Other costs are composed entirely of the SARE expenses which are variable percentages of sales.

Total operating cost is the sum of the variable, fixed, and other costs.

Earnings before taxes are the difference between the revenue and the operating cost.

Income tax is computed as a variable percentage of the earnings before taxes.

Net earnings are the earnings after taxes.

Cash flow is considered as the net earnings plus the depreciation.

Return on investment is calculated as the net earnings divided by the investment.

Payout period is the investment divided by the cash flow.

4. Physical Properties of Components

CHESS-UMR (14) uses critical temperatures, pressures, and volumes throughout all calculations to obtain enthalpies, bubble points, and dew points. The program has sixty-two chemical compounds, called standard chemical components, that may be referred to by number for plants involving these compounds. The program can also handle process networks involving chemical compounds which are not among the standard sixty-two. The required physical and thermodynamic constants used in the Chao-Seader (4) and Yen-Woods (39) correlations must be supplied for these non-standard components. Since the Williams and Otto chemical plant does not use recognizable standard chemical components, non-standard constants are necessary.

The initial assumption for calculation of constants was that the components were paraffin hydrocarbons. The following results were obtained using Maxwell (25):

(1) From molecular weight, the critical pressures were obtained on page 71.

(2) From molecular weight, the normal boiling points were obtained on page 20.

(3) Since the distillation column must operate at approximately 0.5 atmosphere and 100^{o}F, page 42 indicates the normal boiling point of component P must be different from that obtained in (2) above.

(4) With the normal boiling point assumed, the critical temperature was determined on page 69. Designating component A as the heavy key it was determined that component A critical temperature must be decreased by 15^{o}F in order to correspond more closely to the relative volatility of 2.2 specified by Williams and Otto.

(5) The vapor pressure at a reduced temperature of 0.7 for calculation of the accentric factor was obtained for all components on page 42.

(6) The heat of vaporization at the normal boiling point for calculation of the solubility parameter was obtained for all components on page 96.

(7) It was apparent from comparison with the CHESS (27) standard component values that the critical volumes were approximately four times the reciprocal of the density.

The values used are shown in Table XIII.

TABLE XIII

PHYSICAL CONSTANTS

Constant	Component A	B	C	E	P	G
Boiling Point (^oF)	205.0	205.0	490.0	490.0	140.0	690.0
Critical Pressure (psia)	396.0	396.0	241.0	241.0	396.0	160.0
Critical Temperature (^oR)	950.0	965.0	1260.0	1260.0	895.0	1435.0
Critical Volume (cm^3/gm mole)	500.0	500.0	1000.0	1000.0	500.0	1092.0
Molecular Weight (gm/gm mole)	100.0	100.0	200.0	200.0	100.0	300.0
Accentric Factor	0.32067	0.35067	0.61618	0.61618	0.22548	0.78252
Solubility Parameter $(cal/cm^3)^{1/2}$	7.40	7.40	6.10	6.10	6.07	6.73
Molar Volume (cm^3/gm mole)	17.55	17.55	36.80	36.80	17.30	41.10
Heat Capacity (cal/gm mole ^oK)	40.0	40.0	80.0	80.0	40.0	120.0

5. CHESS Representation of Plant 1

Once the physical plan of the CHESS-UMR (14) plant was established, the only variability essentially became the economic subroutine. For plant C1 the reasoning behind the variable selections is given below:

<u>Total Investment</u>

It was found to be almost impossible to obtain plant investments large enough to simulate the $1,035,000 figure reported by Williams and Otto. This caused the return on investment figure calculated by

CHESS-UMR to be so large that the printing format was overloaded with unreasonable values. In order to overcome this problem a location multiplier of 3.5 and a contingency of 10% were used to arrive at the total investment.

Working Capital

The working capital used by Williams and Otto is 31% of their investment plus 10% of sales. In order to correlate the 5% investment figure of CHESS-UMR to this figure, 12% of the sales was used.

Revenue

The only correlation necessary for revenue was to compensate for the inclusion of the waste product.

Variable Costs

The factory indirect costs considered by Williams and Otto were included under variable costs as the operating supplies.

Fixed Costs

In order to correlate all the varied fixed costs the following variables were used:

Labor was 5.95 \$/hr for 8400 hr/yr

Supervision was 20% of labor

Payroll burden was 10% of labor plus supervision

Overhead was 0% of labor

Maintenance was 4.8% of investment to account for repairs

Taxes and insurance were 4.8% of investment to account for laboratory costs

Depreciation was 90% of investment to correspond to Williams & Otto

Interest was 0% of the capital

The overhead and interest were neglected for plant C1 because there was no corresponding value reported by Williams & Otto.

Other Costs

This was made to equal 12.4% by

Sales & Advertising	5.0%
Administration	1.4%
Distribution	1.0%
Research & Development	5.0%

Income Tax

Since Williams and Otto were apparently working with before tax costs the income tax was considered at 0%.

Return on Investment

This value was calculated by Williams and Otto as the net earnings divided by the total fixed plus working capital. CHESS-UMR calculates the value as the net earnings divided only by the investment or fixed capital. It was impossible to reconcile the two values in the CHESS-UMR program so calculations were necessary using the computer output. That is, the total fixed and working capital were added and then divided into the net earnings.

APPENDIX B

EXPERIMENTAL APPARATUS - PLANT 2

1. CHESS-UMR Representation of Plant 2
2. Algebraic Representation of Plant 2

1. CHESS Representation of Plant 2

Plant C2 was designed by the simulation program, CHESS-UMR (14), since the physical plan of the plant was not under investigation, however, the economic variables were all that was varied. The following parameters were inserted to correlate plant C2 to plant C1 as much as possible without disrupting the CHESS-UMR values drastically:

SARE expenses were changed from 34% to 20% to represent a better average value.

Labor was set at 16800 hr/yr to account for two laborers.

Payroll burden was 12% of labor plus supervision since this value was given by Williams and Otto.

Steam and water costs were left at the value specified by Williams and Otto.

The Marshall and Stevens Index for 1959 was used like Williams and Otto.

The plant was allowed to operate for 350 days/yr similar to Williams and Otto.

2. Algebraic Representation of Plant 2

In order to develop as algebraic expression for a plant C2, the internal calculations of CHESS-UMR(14) must be understood.

The overall expression for the return on investment calculated by CHESS-UMR for constant labor cost is:

$$\begin{aligned} ROI = 100*(1 - DNCTX)*[\,&TTPC(1-(ADVAS + ADM \\ &+ OTHRS(8) + ECONO) - OC*DINT) \\ &- DLBR*OTHRS(4)((1 + OTHER)(1 + OTHRS(3)) + OHD + SUPP) \\ &- DNVS(DMAIN + (1 - DEP1)/DEP + TANDI + 1.05\ DINT) \end{aligned}$$

- TTCR - TSTM - TWTR - TELEC]/DNVS

where: (see modified CHESS Users Guide (14) for definitions. The * denotes a factor different from CHESS program.)

DNCTX	=	Income tax	0.500
TTPC	=	Total Sales	Calculated
ADVAS	=	Advertising & Sales	0.1000*
ADM	=	Administration	0.0300*
OTHRS(8)	=	Distribution	0.0200*
ECONO	=	Research & Development	0.0500*
OC	=	Working Capital Factor	0.0835
DINT	=	Interest	0.1000
DLBR	=	General Labor Value	3.5000
OTHRS(4)	=	Labor	16800.0000*
OTHER	=	Supervision	0.2000
OTHRS(3)	=	Payroll Burden	0.1200*
OHD	=	Overhead	0.5000
SUPP	=	Operating Supplies	0.0600
DNVS	=	Total Investment	Calculated
DMAIN	=	Maintenance	0.0500
DEP1	=	Salvage Value	0.1000
DEP	=	Years to Depreciation	11.0000
TANDI	=	Taxes and Insurance	0.0250
TTCR	=	Total Raw Material Cost	Calculated
TSTM	=	Total Steam Cost	Calculated
TWTR	=	Total Water Cost	Calculated
TELEC	=	Total Electric Cost	Calculated
DINDX	=	Marshall & Stevens Cost Index	235.0000*

The calculated values designated above are computed by CHESS-UMR as follows:

$$\mathrm{TTPC} = \sum_{I}^{10,\,15,\,27} \left[\sum_{L=1}^{6} (0.012*\mathrm{DAYS})\mathrm{AMW(L)SEXTSV(L+3,I)} \right] \mathrm{ECOTSV(2,I)}$$

$$\mathrm{DNVS} = 1.214*\mathrm{OTHRS(7)}*(1+\mathrm{COOL})(1+\mathrm{ROADS})\left(\sum_{NE=1}^{18} \mathrm{EOPAR(24,NE)}\right)$$

$$\mathrm{TTCR} = \sum_{I}^{3,\,4} \left[\sum_{L=1}^{6} (0.012*\mathrm{DAYS})\mathrm{AMW(L)SEXTSV(L+3,I)} \right] \mathrm{ECOTSV(2,I)}$$

$$\mathrm{TSTM} + \mathrm{TWTR} + \mathrm{TELEC} = \sum_{NE=1}^{18} \mathrm{EQPAR(23,NE)}$$

where:

DAYS	=	Days per year	350.00*
AMW(L)	=	Molecular Weight	
SEXTSV(L+3,I)	=	Flow rate in lb mole/hr	variable
ECOTSV(2,I)	=	Price of stream $/ton	variable
OTHRS(7)	=	Construction cost factor	1.00
COOL	=	Piping cost	0.02
ROADS	=	Contingency	0.10
EQPAR(24,NE)	=	Installed equipment cost	
EQPAR(23,NE)	=	Utilities costs	
STM	=	Cost of steam	1.00*
WTR	=	Cost of water	0.25*

Collecting terms and consolidating the ROI becomes:

$$ROI = \frac{50[(0.79165)TTPC - 111955.2 - (2.88/11)DNVS - TTCR - utilities]}{DNVS}$$

$$= 50[0.79165(4.2(-20FG + 600FP + 13.60FD)) - 4.2(40FA + 60FB)$$

$$-111955.2 - \Sigma\ EQPAR(23,NE) - (2.88/11)DNVS]/DNVS$$

$$= (99747.9FP + 2260.9524FD - 3324.93FG - 8400FA$$

$$-12600FB - 50\ \Sigma\ EQPAR(23,NE) - 5597760)/$$

$$1.362108\ \Sigma\ EQPAR(24,NE) \qquad -(144/11)$$

Since the distillation tower is the major contributing factor in the plant at 25% of the total investment, both the utilities and investment should be proportional to the flow rate into the tower.

The final form of the algebraic representation for plant A2 becomes:

$$ROI = \frac{(P'*FP + D'*FD - G'*FG - A'*FA - B'*FB - U'*FR - C')}{(E'*FR)} - CC'$$

where:

A'	=	8400
B'	=	12600
C'	=	5597760
D'	=	2260.9524
G'	=	3324.93
P'	=	99747.9
CC'	=	144/11
E'	=	Determined experimentally
U'	=	Determined experimentally. The value determined must be 50 times the sum of the utilities costs.

APPENDIX C

COMPUTER PROGRAMS

1. Fortran IV - (G)
2. CPS PL-1

1. Fortran IV - (G)

The following computer programs were written or modified for use in Fortran IV at the University of Missouri-Rolla on an IBM 360-50.

a. Algorithm II-T was modified from the Ph.D. dissertation of James H. Christensen, University of Wisconsin, 1969. The original program was written in Fortran II and produces a solution procedure, for a system of equations, which requires the minimum assumptions.

b. Surface was written to provide a direct search of the surface under investigation in the present thesis.

c. CHESS was compiled and modified to provide an economic evaluation of the chemical plant under investigation.

d. Davidon-Fletcher & Powell was modified from Ferguson to provide a formal optimization technique. The modification included addition of constraint capabilities and evaluation of the objective function with derivatives.

e. Hooke & Jeeves-Wood was modified from Weisman et al. (35) to include the constraints and evaluation of the objective function for an additional formal optimization technique.

2. CPS PL-1

The following computer programs were written in PL-1 for use on an IBM 2741 remote terminal coupled with the IBM 360-50 at the University of Missouri-Rolla.

a. MASS evaluates a complete mass balance including all flow rates in pounds per hour for plant A1.

b. MOLE evaluates a complete mass balance including all flow rates in moles per hour for plant A1.

c. SOLVZ evaluates the objective function for plant A1.

d. CHESOL evaluates the objective function for plant A2.

e. ZITER provides a direct search routine for plant A1 as FRE, FRC, TX, and PHI vary.

f. CHESIT provides a direct search routine for plant A2 as FRE, FRC, TX, and PHI vary.

g. WOODOP is used in conjunction with subroutines to optimize the objective function by the Hooke and Jeeves method.

APPENDIX D

NUMERICAL RESULTS

The constraint method of Gottfried, Bruggink and Harwood (16) was used on all formal optimization techniques attempted in this study. A summary of the reasoning behind the selection of various factors, therefore, is appropriate.

Assume a sample optimization problem:

Object = optimum $Y(\bar{X})$

Subject to: $H_j(\bar{X}) = 0 \quad j = 1,2,\text{---}l;\ l < N$

$H_j(\bar{X}) \leq 0 \quad j = l+1,\ l+2,\text{---}m$

$a \leq \bar{X} \leq c$

Produce a modified objective function

$$z(\bar{x},d_1,d_2) = y(\bar{x}) \pm (d_1 w_1(\bar{x}) + (1/d_2) w_2(x)) \begin{cases} + \text{ for maximum} \\ - \text{ for minimum} \end{cases}$$

where: $w_1(\bar{x}) = \sum_{j=1}^{l} b_j H_j^2(\bar{x}) + \sum_{j=l+1}^{m} b_j g_j H_j^2(\bar{x})$ (Exterior)

$$w_2(\bar{x}) = \sum_{i=1}^{N} \left[\frac{1}{c_i - x_i} + \frac{1}{x_i - a_i} \right] \qquad \text{(Interior)}$$

$$g_j = \begin{cases} 0 & \text{IF } H_j(\bar{x}) \leq 0 \\ 1 & \text{IF } H_j(\bar{x}) > 0 \end{cases} \quad j = l+1,\ l+2,\text{---}m$$

d_1 and $d_2 > 0$ are scalar penalty coefficients

$b_i > 0,\ i = 1,\ 2,\text{---}m$ are scalar scale factors to avoid dominance by any constraint.

The procedure of use is to choose d_1 and d_2 and optimize z. Then increase d_1 and d_2 and again optimize z. This is continued until the d's have become sufficiently large and the constraints are satisfied to some tolerance.

For the problem in this study, the following values are assigned to maximize z with the minimizing routines used:

$z(\bar{x}) = z$ (FRE,FRC,TX,PHI)

Subject to:

$FRE \geq 0$	or	$H_1 = -FRE \leq 0$
$FRC \geq 0$	or	$H_2 = -FRC \leq 0$
$580 \leq TX \leq 680$	or	$H_3 = 580 - TX \leq 0,\ H_4 = TX - 680 \leq 0$
$1 - PHI \geq 0$	or	$H_5 = PHI - 1 \leq 0$
$PHI \geq 0$	or	$H_6 = -PHI \leq 0$
$12400 \leq FA \leq 16600$	or	$H_7 = 12400 - FA \leq 0,\ H_8 = FA - 16600 \leq 0$
$R3 \geq 0$	or	$H_9 = -R3 \leq 0$
$z \geq 0$	or	$H_{10} = -z \leq 0$

The modified objective function becomes:

$$y = d_1 w_1(\bar{x}) + (1/d_2)\ w_2(\bar{x}) - z$$

where:

$$w_1(\bar{x}) = \sum_{j=1}^{10} b_j g_j H_j^2(\bar{x})$$

$w_2(\bar{x}) = 0$ since the problem has been constructed with no bounds on the independent variables. Thus, d_2 is unnecessary.

The following reasoning was used to determine the scale factor b_j, $j = 1,2,$---10.

Constraint Equation	Probable Variation	Square	Scale Factor
$H_1 = -FRE$	100	10000	0.001
$H_2 = -FRC$	100	10000	0.001
$H_3 = 580 - TX$	10	100	0.1
$H_4 = TX - 680$	10	100	0.1
$H_5 = PHI - 1$	0.1	0.01	1000
$H_6 = -PHI$	0.1	0.01	1000
$H_7 = 12400 - FA$	10	100	0.1
$H_8 = FA - 16600$	10	100	0.1
$H_9 = -R3$	10	100	0.1
$H_{10} = -z$	1	1	1

The following summary shows the results of the Hooke and Jeeves search routine on both plant A1 and plant A2 when started at four different points.

Plant A1

d_1	Iteration	FRE	FRC	TX	PHI	z	Remarks
	1	100000	500	585	0.7000	-10.25	Arbitrary
10^{-6}	658	151607	8076	675	0.0962	123.08	
10^{-3}	1270	148432	7888	674	0.0983	123.18	
1	2201	151767	8035	674	0.0961	123.07	
10^3	2248	18055	1009	588	0.6950	-20.35	Time>3 min
	1	60542	3331	656	0.2463	73.34	DS
10^{-6}	364	144213	7735	674	0.1011	123.20	
10^{-3}	728	144213	7735	674	0.1011	123.20	
1	1092	144213	7735	674	0.1011	123.20	
10^3	1456	144213	7735	674	0.1011	123.20	
10^6	1820	144213	7735	674	0.1011	123.20	
	1	60677	3420	636	0.2390	55.16	AS
10^{-6}	522	145214	7736	674	0.1004	123.21	
10^{-3}	1013	141723	7621	674	0.1029	123.15	
1	1504	141723	7621	674	0.1029	123.15	
10^3	1994	141723	7621	674	0.1029	123.15	
10^6	2267	120924	6983	669	0.1208	119.89	Time>3 min
	1	111314	7065	657	0.1296	108.00	HR
10^{-6}	284	143290	7675	674	0.1018	123.19	
10^{-3}	568	143290	7675	674	0.1018	123.19	
1	852	143290	7675	674	0.1018	123.19	
10^3	1136	143290	7675	674	0.1018	123.19	
10^6	1420	143290	7675	674	0.1018	123.19	

Plant A2

d_1	Iteration	FRE	FRC	TX	PHI	z	Remarks
	1	100000	500	585	0.7000	-4580.53	Arbitrary
10^{-6}	206	18055	10	581	0.5878	2.89E9	R3 = -1035
10^{-3}	740	22375	1040	571	0.6914	1173.71	FA = 11703
1	1475	24375	1479	579	0.6309	1076.90	
10^{3}	1683	27163	10	579	0.7009	556.02	
10^{6}	1934	27163	10	580	0.7009	556.00	
	1	60542	3331	656	0.2463	61.59	DS
10^{-6}	632	21691	10	579	0.6879	1601.31	FA = 8689
10^{-3}	1397	22623	1053	579	0.6838	1173.42	FA = 11704
1	2259	64233	3557	579	0.2434	678.11	Time>3 min
	1	60677	3420	636	0.2390	229.60	AS
10^{-6}	689	21922	10	579	0.6803	1601.43	FA = 8683
10^{-3}	1390	23052	1088	579	0.6701	1171.41	FA = 11717
1	2279	51693	3308	580	0.2945	794.69	Time>3 min
	1	111314	7065	657	0.1296	61.52	HR
10^{-6}	325	15889	9	581	0.6624	2.62E9	R3 = -1104
10^{-3}	1134	22572	1046	579	0.6857	1173.77	FA = 11702
1	2115	114055	6433	580	0.1366	417.68	Time>3 min